PCT

WORLD INTELLECTUAL PROPERTY ORGANIZATION
International Bureau

INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification 6 : G06F 159:00

A1

(11) International Publication Number: WO 97/41526

(43) International Publication Date: 6 November 1997 (06.11.97)

(21) International Application Number: PCT/US97/07218

(22) International Filing Date: 28 April 1997 (28.04.97)

(30) Priority Data:
08/641,071 26 April 1996 (26.04.96) US

(71) Applicant: THE SCRIPPS RESEARCH INSTITUTE [US/US]; 10666 North Torrey Pines Road, La Jolla, CA 92037 (US).

(72) Inventors: WILSON, Ian, A.; 1025 Newkirk Drive, La Jolla, CA 92037 (US). LIVNAH, Oded; 5240 Fiore Terrace #3114, San Diego, CA 92122 (US). STURA, Enrico, A.; 5172 Park West Avenue, San Diego, CA 92117 (US). JOHNSON, Dana, L.; 1343 Lonely CoHage Road, Upper Black Eddy, PA 18972 (US). JOLLIFFE, Linda, K.; 16 Davenport Way, Belle Mead, NJ 08502 (US).

(74) Agent: LAND, John; Fish & Richardson, P.C., 4225 Executive Square, Suite 1400, La Jolla, CA 92037 (US).

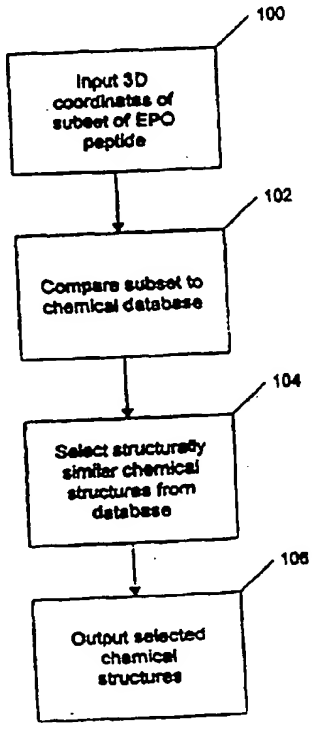
(81) Designated States: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, ARIPO patent (GH, KE, LS, MW, SD, SZ, UG), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG).

Published
With international search report.

(54) Title: SMALL MOLECULE MIMETICS OF ERYTHROPOIETIN

(57) Abstract

The invention features computer-assisted methods (100, 102, 104, 106, 200, 202, 204) for identifying molecules which will bind to the EPO receptor and act as an erythropoietin (EPO) mimetic. Preferred EPO mimetics identified using the method of the invention act as agonists of the EPO receptor in one or more *in vitro* or *in vivo* biological assays of EPO activity.



FOR THE PURPOSES OF INFORMATION ONLY

Codes used to identify States party to the PCT on the front pages of pamphlets publishing international applications under the PCT.

AL	Albania	ES	Spain	LS	Lesotho	SI	Slovenia
AM	Armenia	FI	Finland	LT	Lithuania	SK	Slovakia
AT	Austria	FR	France	LU	Luxembourg	SN	Senegal
AU	Australia	GA	Gabon	LV	Latvia	SZ	Swaziland
AZ	Azerbaijan	GB	United Kingdom	MC	Monaco	TD	Chad
BA	Bosnia and Herzegovina	GE	Georgia	MD	Republic of Moldova	TG	Togo
BB	Barbados	GH	Ghana	MG	Madagascar	TJ	Tajikistan
BE	Belgium	GN	Guinea	MK	The former Yugoslav Republic of Macedonia	TM	Turkmenistan
BF	Burkina Faso	GR	Greece	ML	Mali	TR	Turkey
BG	Bulgaria	HU	Hungary	MN	Mongolia	TT	Trinidad and Tobago
BJ	Benin	IE	Ireland	MR	Mauritania	UA	Ukraine
BR	Brazil	IL	Israel	MW	Malawi	UG	Uganda
BY	Belarus	IS	Iceland	MX	Mexico	US	United States of America
CA	Canada	IT	Italy	NE	Niger	UZ	Uzbekistan
CF	Central African Republic	JP	Japan	NL	Netherlands	VN	Viet Nam
CG	Congo	KE	Kenya	NO	Norway	YU	Yugoslavia
CH	Switzerland	KG	Kyrgyzstan	NZ	New Zealand	ZW	Zimbabwe
CI	Côte d'Ivoire	KP	Democratic People's Republic of Korea	PL	Poland		
CM	Cameroon	KR	Republic of Korea	PT	Portugal		
CN	China	KZ	Kazakstan	RO	Romania		
CU	Cuba	LC	Saint Lucia	RU	Russian Federation		
CZ	Czech Republic	LI	Liechtenstein	SD	Sudan		
DE	Germany	LK	Sri Lanka	SE	Sweden		
DK	Denmark	LR	Liberia	SG	Singapore		
EE	Estonia						

SMALL MOLECULE MIMETICS OF ERYTHROPOIETIN

BACKGROUND OF THE INVENTION

1. *Field of the Invention*

This invention relates to computer-assisted methods for identifying and designing small molecule mimetics of erythropoietin.

2. *Description of Related Art*

Erythropoietin (EPO) is the primary regulator of the proliferation and differentiation of immature erythroid cells. EPO is produced in the fetal liver and in the adult kidney in response to hypoxia (low oxygen levels in blood or tissue). It circulates in the blood stream where it targets the EPO receptor (EPOR) on committed progenitor cells in the bone marrow and other hematopoietic tissues. Recombinant human erythropoietin (rHuEPO) is widely used in therapy of patients with anaemia due to chronic renal failure, cancer chemotherapy and AZT treatment.

The EPO receptor belongs to the cytokine receptor superfamily, which includes receptors for other hematopoietic growth factors such as interleukins (ILs), colony stimulating factors (CSFs) as well as growth hormone prolactin and ciliary neurotrophic factor (CNTF). The structural architecture of this family of receptors consists of three modules: a ligand binding extracellular domain, a short trans membrane region and a large cytoplasmic domain. It has been proposed that the extracellular domain of this superfamily comprises two discrete domains each containing approximately 100 residues that fold into a sandwich consisting of 7 antiparallel β-strands with the topology of an Ig constant domain. Members of the family share two characteristic motifs in their extracellular domain: a pair of conserved disulfide bridges in the N-terminal domain, and a WSXWS box (where X is any amino acid residue) in the C-terminal domain. For most members of this receptor superfamily, oligomerization of one or more polypeptide chains

is essential for forming high affinity receptor complexes. A homodimer complex has been demonstrated to be the active form of hGHR and a similar model has been suggested for G-CSF, prolactin and EPO receptors.

Erythropoietin induces dimerization of two EPO receptor molecules, which results in subsequent phosphorylation of the cytoplasmic domains by the association with two tyrosine kinase (JAK2) molecules to initiate a cascade of events that leads to the relevant biological.

Given the importance of erythropoietin, it would be very desirable to be able to identify molecules capable of binding the EPO receptor and eliciting the response normally elicited by EPO.

SUMMARY OF THE INVENTION

The invention features methods for identifying molecules which will bind to the EPO receptor and act as a EPO mimetic. Preferred EPO mimetics identified using the method of the invention act as agonists of the EPO receptor in one or more *in vitro* or *in vivo* biological assays of EPO activity. Preferred mimetics are molecules lacking peptide bonds, i.e., are non peptidic mimetics. Preferred peptide mimetics have 15 or fewer, more preferably 10 or fewer amino acids.

The methods of the invention entail identification and design of molecules having a particular structure. The methods rely on the use of precise structural information derived from x-ray crystallographic studies of the extracellular domain of EPO receptor (amino acids 1 to 225) complexed with a peptide, EMP1 (EPO Mimetic Peptide 1; described below), which acts as an EPO mimetic. This crystallographic data permits the identification of atoms in the peptide mimetic that are important for EPO receptor binding and dimerization. More importantly, this data defines a three dimensional array of the important contact atoms. Other molecules which include a portion in which the atoms have a similar three dimensional arrangement similar to some or all of these contact atoms are likely to be capable of acting as an EPO mimetic. Moreover, one can use the structural information to design or identify molecules having even more EPO activity than the peptide mimetic described herein.

The details of the preferred embodiment of the present invention are set forth in the accompanying drawings and the description below. Once the details of the invention are known, numerous additional innovations and changes will become obvious to one skilled in the art.

BRIEF DESCRIPTION OF THE DRAWINGS

FIGURE 1 is a flowchart showing a first method for identifying potential mimetics of erythropoietin using a computer system.

FIGURE 2 is a flowchart showing a second method for identifying potential mimetics of erythropoietin using a computer system.

Like reference numbers and designations in the various drawings indicate like elements.

DETAILED DESCRIPTION OF THE INVENTION

Throughout this description, the preferred embodiment and examples shown should be considered as exemplars, rather than as limitations on the present invention.

Described below is the crystal structure of a small peptide mimetic of EPO bound to an extracellular portion of the EPO receptor. The peptide, EMP1 (GGTYSCHFGPLTWVCKPQGG; SEQ ID NO:1), is characterized by an intramolecular disulfide bridge. Several lines of evidence suggest that EMP1 can act as an EPO mimetic. For example, EMP1 competes with EPO in receptor binding assays and induces cellular proliferation of cell lines engineered to be responsive to EPO. Both EPO and peptide induce a similar cascade of phosphorylation events and cell cycle progression in EPO responsive cells. Furhter, EMP1 demonstrates significant erythropoietic effects in mice as monitored by two different *in vivo* assays of nascent red blood cell production. This data, when combined, strongly supports the notion that the peptide ligand, which has a sequence unrelated to that of EPO, is capable of binding to and inducing an agonist conformation or assembly of EPO receptor.

Design of small molecule mimetics

The structure of the EMP1 dimer demonstrates that a molecule substantially smaller than the natural hormone can act as an agonist and induce the appropriate biological response. The peptide is assumed to have a substantially smaller contact interface with the receptor than its natural hormone. The binding determinants in the EPO receptor form an almost flat surface which is mainly hydrophobic in nature, without any cavities or charged residues that may help in design of a small molecule ligand to interact with the receptor.

This simplified framework of interactions revealed by the structural data presented herein can be used to identify additional EPO mimetics. The atoms of EMP1 which are important for binding to the EPO receptor and forming dimeric EPO receptor include those involved in the contact between the EMP1 (peptide) and EBP (EPO receptor) and

those involved in contacts between the two EMP1 molecules in the dimeric complex (peptide-peptide contacts). In addition to the contacts listed in Table 2, the following EMP1-EMP1 hydrophobic contacts are significant: Tyr^{P4}, Cys^{P6}, Phe^{P8}, Trp^{P13}, and Cys^{P15} in each peptide. The following EMP1-EBP hydrophobic interactions are also significant: Tyr^{P4}, Phe^{P8}, and Trp^{P13} in each peptide. It will be understood by those skilled in the art that not all of the atoms present in a significant contact residue need be present in a mimetic. In fact, it is only those few atoms which actually from important contacts with the EPO receptor which are likely to be important for mimetic activity. Those skilled in the art will be able to identify these important atoms based on the model of the dimeric EMP1-EPO complex which can be constructed using the structural data herein.

Preferred mimetics will include atoms at postions similar to those of the EPO receptor contacting atoms of EMP1. Even more preferred mimetics will be structurally similar to the dimer of EMP1 found in the structure described below. This is because the dimerization of EMP1 is an important factor in the diemerization of the EPO receptor.

The methods of the invention employ a computer-based methods for identifying compounds having a desired structure. More specifically, the invention uses the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the human EPO receptor, to determine peptide and non-peptide mimetic candidates by means of computer methods.

These computer-based methods fall into two broad classes: database methods and *de novo* design methods. In database methods the compound of interest is compared to all compounds present in a database of chemical structures and compounds whose structure is in some way similar to the compound of interest are identified. The structures in the database are based on either experimental data, generated by NMR or x-ray crystallography, or modeled three-dimensional structures based on two-dimensional (*i.e.*, sequence)

data. In *de novo* design methods, models of compounds whose structure is in some way similar to the compound of interest are generated by a computer program using information derived from known structures, *e.g.*, data generated by x-ray crystallography and/or theoretical rules. Such design methods can build a compound having a desired structure in either an atom-by-atom manner or by assembling stored small molecular fragments.

The success of both database and *de novo* methods in identifying compounds with activities similar to the compound of interest depends on the identification of the functionally relevant portion of the compound of interest. For drugs, the functionally relevant portion is referred to a pharmacophore. A pharmacophore then is an arrangement of structural features and functional groups important for biological activity, *e.g.*, EPO activity.

Not all identified compounds having the desired pharmacophore will act as an EPO mimetic. The actual activity can be finally determined only by measuring the activity of the compound in relevant biological assays. However, the methods of the invention are extremely valuable because they can be used to greatly reduce the number of compounds which must be tested to identify an actual mimetic.

Dimerization of the EPO receptor is important for activity. Accordingly, preferred mimetics will be based on the structure of the EMP1 dimer as it is bound to the EPO receptor dimer. Thus, preferred mimetics have include important contacts from both of the RWJ 61233 peptides present in the structure described below. Such mimetics will favor dimerization of the EPO receptor.

Programs suitable for generating predicted three-dimensional structures from two-dimensional data include: Concord (Tripos Associated, St. Louis, MO), 3-D Builder (Chemical Design Ltd., Oxford, U.K.), Catalyst (Bio-CAD Corp., Mountain View, CA), and Daylight (Abbott Laboratories, Abbott Park, IL).

Programs suitable for searching three-dimensional databases to identify molecules bearing a desired pharmacophore include: MACCS-3D and ISIS/3D (Molecular Design Ltd., San Leandro, CA), ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.), and Sybyl/3DB-Unity (Tripos Associates, St. Louis, MO).

Programs suitable for pharmacophore selection and design include: DISCO (Abbott Laboratories, Abbott Park, IL), Catalyst (Bio-CAD Corp., Mountain View, CA), and ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.).

Databases of chemical structures are available from Cambridge Crystallographic Data Centre (Cambridge, U.K.) and Chemical Abstracts Service (Columbus, OH).

De novo design programs include Ludi (Biosym Technologies Inc., San Diego, CA) and Aladdin (Daylight Chemical Information Systems, Irvine CA).

Those skilled in the art will recognize that the design of a mimetic may require slight structural alteration or adjustment of a chemical structure designed or identified using the methods of the invention.

In general, chemical compounds identified or designed using the methods of the invention can be sythesized chemically and then tested for EPO activity using any of the methods described below. The methods of the invention are particularly useful because they can be used to greatly decrease the number potential mimetics which must be screened for EPO activity.

The invention may be implemented in hardware or software, or a combination of both. However, preferably, the invention is implemented in computer programs executing on programmable computers each comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions

described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

Each program is preferably implemented in a high level procedural or object oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

Each such computer program is preferably stored on a storage media or device (*e.g.*, ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The inventive system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

FIGURE 1 is a flowchart showing a first method for identifying potential mimetics of erythropoietin using a computer system. The method uses a programmed computer comprising a processor, a data storage system, at least one input device, and at least one output device, and comprises the steps of:

(1) inputting into the programmed computer through an input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the receptor, thereby generating a criteria data set (STEP 100);

(2) comparing, using the processor, the criteria data set to a computer database of chemical structures stored in the computer data storage system (STEP 102);

(3) selecting from the database, using a program suitable for searching three-dimensional databases to identify molecules bearing a desired pharmacophore (such as those described above or equivalents), chemical structures having a portion that is structurally similar to the criteria data set (STEP 104);

(4) outputting to an output device the selected chemical structures having a portion similar to the criteria data set (STEP 106).

FIGURE 2 is a flowchart showing a second method for identifying potential mimetics of erythropoietin using a computer system. The method uses a programmed computer comprising a processor, a data storage system, at least one input device, and at least one output device, and comprises the steps of:

(1) inputting into the programmed computer through an input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the receptor, thereby generating a criteria data set (STEP 200);

(2) constructing, using a program suitable for generating chemical structure models (such as those described above or equivalents), a model of a chemical structure having a portion that is structurally similar to the criteria data set (STEP 202);

(3) outputting to the output device the constructed model (STEP 204).

Confirmation of Biological Activity

In order to determine whether a molecule identified using the methods of the invention can act as an EPO mimetic, one or more *in vitro* or *in vivo* assays of EPO activity should be performed. For example, mimetic molecules should be able to stimulate proliferation of TF-1 cells (Kitamura et al., J. Cell Physiol. 140:323, 1985) or B6Sut cells (Greenberger et al., Proc. Natl. Acad. Sci. USA 80:2931, 1983), but preferably do not stimulate proliferation of cells which do not bear the EPO receptor. Thus, preferred mimetics do not stimulate proliferation of Mo7e cells (Avanzi et al., Br. J. Haematol. 69:359, 1988).

Potential mimetics can also be tested in a murine model of erythropoiesis. In this assay a potential mimetic is administered to normal mice which express endogenous basal levels of EPO. Reticulocytes are counted, preferably by flow cytometry, to determine whether the candidate mimetic increases reticulocyte levels. An increase in reticulocyte levels indicates that the candidate mimetic is stimulating erythropoiesis. Because the mice used in this assay already express EPO, this assay may be relatively insensitive. As an alternative, candidate mimetics can be assayed in the exhypoxic-polycythemic mouse bioassay. In this assay polycythemia is induced by conditioning mice in a hypobaric chamber to reduce endogenous EPO levels. A potential EPO mimetic can be administered to a conditioned mouse. Incorporation of ^{59}Fe into blood serves as a measure of erythropoiesis. This erythropoiesis can be attributed to the candidate mimetic.

The assays described above are examples of suitable assays. Other assays for EPO activity known to those skilled in the art are also useful.

In order to determine the biological activity of a candidate mimetic it is preferable to measure biological activity at several concentrations of candidate mimetic. The activity at a given concentration of candidate mimetic can be compared to the activity of EPO itself.

Structural Data

The coordinates for amino acids 1 to 225 of the human EPO receptor bound to peptide EMP1 are presented in the attached appendix in standard Brookhaven database format. Also included in this appendix is a list of van der Waals interactions. These coordinates can be used in the design and identification of EPO mimetics according to the methods of the invention.

Structure of EBP-EMP1 Complex

The extracellular fragment of human EPO receptor (EPO binding protein, EBP), consisting of residues 1-225, was expressed in Escherichia coli and purified as described

(Johnson et al., Protein Express. Purif. 7:104, 1996). Rhomboidal-shaped crystals of an EBP complex with EMP1 were obtained in orthorhombic space group $P2_12_12_1$, with cell parameters a=59.2Å, b=75.5Å, c=132.2Å, with two EBP and two peptide molecules in the asymmetric unit and a V_M=2.8 Å³/dalton (Matthews, J. Mol. Biol. 33:491, 1968). The crystal structure was determined by multiple isomorphous replacement (MIR) using two heavy atom derivatives (Table 1). Residues 1-2 and 19-20 of each peptide as well as residues 1-9, 21-23, 164-166, 221-225 of receptor molecule I, and residues 1-9, 21-23, 133-135, 221-225 of receptor molecule II had poor or no electron density and are excluded from the structure analyses

An important break in the electron density that affects the structure interpretation occurs for the three residues (Arg^{21} -Gly^{22} -Pro^{23}) that link the amino terminal α-helix to the first β-strand in D1 of both receptor molecules. A molecular packing diagram shows the proximity of a second non-crystallographically related dimer in the crystal that gives two possibilities of how this three-residue linker may be connected. The current choice of linker connectivity is based on a structure of another independent EBP-peptide complex at higher resolution (2.5 Å), which shares a similar molecular packing, but for which the electron density is clear for these three residues. At present there are no experimental data to verify whether this N-terminal α-helix exists in solution or is a crystallization packing artifact. Notably, this helical region is not observed in the published structures of hGHbp (begins at residue 32; deVos et al., Science 255:306, 1992), PRLR (begins at residue 2, without any defined secondary structure until the first β-strand, residue 6; Somers et al., Nature 372:478, 1994), the INF-γRα (begins at residue 17; Walter et al., Nature 376:230, 1995) or the tissue factor (begins at residue 3 without any defined secondary structure until the first β-strand, residue 11; Muller et al., Nature 370:662, 1994).

The EBP monomer folds into two domains, D1 and D2, that form an L-shape with the long axis of each domain aligned at approximately 90° to each other; the overall molecular dimensions are 45 Å x 52 Å x 62 Å. The N-terminal domain (D1, residues 10-

114) and C-terminal domain (D2, residues 119-220) are connected by a short four residue α-helix linker. Both domains are more closely related in overall topology to Fibronectin type-III (FBN-III) domains than to Ig domains (Bork et al., J. Mol. Biol., 242:309, 1994). The FBN-III fold is composed of two antiparallel β-pleated sheets, consisting of strands A, B, E and strands G, F, C and C', and is found in the two domains of the human growth hormone (de Vos et al., Science 255:306, 1992) and prolactin (Somers et al., Nature 372:478, 1994) receptors, the D1 and D2 domains of the α chain of interferon-γ receptor (IFN-γRα) (Walter et al., Nature 376:230, 1995), the D2 domain of CD4 (Wang et al, Nature 348:411, 1990; Ryu et al., Nature 348:419, 1990), the two domains of tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994), the third fibronectin-type repeat of tenacin (Leagy et al., Science 258:987, 1992) and the D2 domain of the chaperone protein PapD (Holmgren et al., Nature 342:248, 1989). The FBN-III topology differs from an Ig constant domain by a shift of strand D from one β-sheet (strands A, B, E and D) to the other (strands G, F, C, C'), where it is defined as the C' strand. Superposition of equivalent β-sheet core residues of the D1 and D2 domains in EBP gives an r.m.s. deviation of 2.3 Å for 77 Cα pairs, which is significantly larger than the corresponding domain overlaps for hGHbp (1.1Å) and PRLR (0.8Å), and reflects a difference in the subclass of fold between the two EBP domains.

In D1, a short α-helix (residues 10-20), precedes the first β-sandwich that is better described as a hybrid of the FBN-III fold with an Ig fold (residues 24-114), rather than strict FBN-III topology. In this h-type fold (Wang et al., Nature 348:411, 1990; Ryu et al., Nature 348:419, 1990), the C' strand is long and interacts first with strand C and then switches to interact with strand E (where C' changes its designation to strand D) forming a four-on-four strand β-sandwich. D1 contains the two conserved disulfide bridges linking Cys^{26} (βA) to Cys^{36} (βB) and Cys^{47} (βC') to Cys^{82} (βE). The number of residues between the cysteine pairs that form the two disulfide bridges are 9 and 15 for EBP, compared to 9 and 10 in both GHR and PRLR. The longer connection between strands C' and E enables the second half of strand C' to become strand D. This h-type topology is not found in either of the two s-type GHR domains. A potential glycoylation site exists

on residue Asn^{52} which is located towards the end of the loop region connecting the βB and βC strands. Although Asn^{52} is not glycosylated in this bacterially expressed protein, an external cavity around the Asn^{52} side chain could easily accommodate a carbohydrate moiety.

A helical linker (residues 115-118) connects D1 to D2 (The ϕ, Ψ torsion angles for the interdomain helical linker for Ile^{115}, Asn^{116}, Glu^{117} and Val^{118} are -50° -27°, -76°, -21°, -99°, 26°, and -151°, 38° respectively.) and has been observed in other members of this receptor family, hGHbp, PRLR, IFN-γRα and tissue factor. In EBP, the domain association is further restricted by a mixed assortment of hydrogen bonding, hydrophobic interactions and one salt bridge (between Arg^{21} and Asp^{122}) from 11 residues of D1 and 12 residues of D2 with a total buried surface [The molecular surface areas buried by interaction were calculated using the program MS (Connolly, J. Appl. Crystallog, 16:439, 1983) using a 1.7Å probe sphere and standard atomic radii (as described in Davies, et al, Ann. Rev. Biochem. 59:439, 1990). There may be some discrepancies between values reported here and other (deVos et al., Scince 255:306, 1992) published values due to use of a different algorithm (Connolly) vs. Lee et al., J. Mol. Biol., 55: 379, 1971) and probe radii. For clarity all values reported here have been calculated in the same way for better comparison between the receptors] of 950 $Å^2$ for the two domains.

D2 (residues 119-220) folds into the standard FBN-III (s-type) topology with one free cysteine and no disulfide bridges, consistent with GHR and PRLR that have three and two disulfide bridges, respectively, in D1 but none in D2. After the α-helix linker, D2 begins with an irregular coil (residues 118-126) that contains Pro^{124} which is conserved in the structures of hGHbp, PRLR, tissue factor and IFNγ-Rα, and based on sequence alignment, in most class-1 and class-2 cytokine receptors (Bazan, Proc. Natl. Acad. Sci. USA 87:6934, 1990). This short coil ends with Gly^{124} which has a positive ϕ (ϕ, Ψ ≈ 52°,40°) consistent with the equivalent Ala^{136} and Ala^{101} torsion angles in hGHbp (ϕ, Ψ ≈ 63°,68°) and PRLR (ϕ, Ψ ≈ 58°,38°). The Pro^{124} region forms an analogous extended bulge conformation adjacent and parallel to a corresponding bulge containing the

WSXWS motif. The WSAWS sequence forms a modified wide β-bulge (Richardson, Adv. Prot. Chem. 34:167, 1981) and is located in an extended chain region immediately preceding the βG strand that would normally connect to the membrane spanning region of the EPOR.

The quaternary structure of the complex is composed of two peptides and two receptors that form a T-shapes assembly. A noncovalent peptide dimer interacts with two receptor molecules to generate an almost perfect 2-fold symmetrical arrangement. After superposition of D2 of the two EBP molecules in the dimer, the centers of mass of the two D1 domains are only 0.8 Å apart, sufficient to perturb perfect two-fold symmetry. Separate superposition of the corresponding D1 and D2 of each receptor in the dimer results in r.m.s. deviations of 0.53 Å (105 D1 Cα pairs) and 0.47 Å (93 D2 Cα pairs).

The cyclic EMP1 contains a single disulfide bridge between Cys^{P6} and Cys^{P15}, which links two short β-strands (residues 4-7 and 13-16) that are connected by a slightly distorted type 1 β-turn [Pro^{P10} (i+1) and Leu^{P11} (i+2) of the β-turn have $\phi,\Psi \approx -62°$, -38° and -99°, -60°, respectively. The carbonyl oxygen of Leu^{P11} has a hydrogen bond to EBP distorting the Ψ value from its normal 0°±30° (i+2) in a standard type I β-turn.] consisting of residues Gly^{P9}-Pro^{P10}-Leu^{P11}-Thr^{P12}. Each peptide has a very close association with its other peptide partner and buries 320 Å of its 1220 $Å^2$ molecular surface in this interaction (Connelly, J. Appl. Crystallog. 16:439, 1983; Davies et al., Ann. Rev. Biochem. 59:439, 1990; Richards, J. Mol. Biol. 55:379, 1971). Four hydrogen bonds between the mainchains of the two peptides results in formation of a four-stranded anti-parallel β-pleated sheet (Table 2). Two symmetric hyrdophobic cores are assembled by peptide dimerization and are comprised of the disulfide bridges and the side chains of Tyr^{P4},Phe^{P8} and Trp^{P13}. The construction of each hydrophobic core resembles a box which places the aromatic rings of Phe^{P8},Trp^{P13} and Tyr^{P4} (from the other peptide) and the disulfide bridge (Cys^{P6}-Cys^{P15}) at the corners. The two glycine residues at either end of the peptide are not structured.

The peptide dimer is embedded in a deep crevice between two EBP receptor molecules. A portion of each peptide monomer interacts with both receptor molecules. The binding sites of each EBP are practically identical due to the 2-fold symmetric interactions imposed on binding the peptide dimer. The four major contact areas on EBP come from segments on four loop regions (L1, L3, L5, L6) that connect strands A to B (L1 residues 33-34) and F to G (L6 residues 90-94) in D1 and strands B to C (L5 residues 148-153) and F to G (L6 residues 203-205) in D2. The total buried molecular surfaces in the peptide-EBP assembly are 840 $Å^2$ and 880 $Å^2$ for the two peptides and EBP's, respectively. The peptide-EBP interaction can be separated into distinct hydrophobic (67%) and polar (33%) areas. A hydrophobic core is formed between the peptide and receptor and comprises Phe^{93},Met^{150} and Phe^{205} from one EBP molecule and the peptide hydrophobic box consisting of Phe^{P8} and Trp^{P13} from one peptide and Tyr^{P4} and Cys^{P15} from the other peptide. The polar interactions are located mainly at the bottom of the binding crevice and are mainly with loop L5 in D2. Five of the six hydrogen bonds are between the mainchain of the β-turn residues Gly^{P9},Pro^{P10} and Leu^{P11} from one peptide with the mainchain and sidechain hydroxyl of conserved Tyr^{P4}, which crosses over its other peptide partner, to interact with loop L3 (Table 2). The EBP-EBP interaction makes a surprisingly minor contribution to the overall stability of the complex where the inter-receptor buried molecular surface is only 75 $Å^2$, contributed by Leu^{175} and Arg^{178} from each receptor molecule.

EMP1 is one of a family of sequences that contain several conserved residues, besides the cysteines ([redacted]). The most structurally significant of these consensus residues appear to be Tyr^{P4} and Trp^{P13}, which along with the disulfide bridge have a major contribution to the hydrophobic core of the peptide-peptide interaction. Moreover, these two aromatic residues play a pivotal role in peptide-receptor interaction and in receptor dimerization.

Dimerization of EBP in Solution

To explore the interaction of EMP1 with EBP in solution we employed a bifunctionalsulphydryl reactive crosslinker DPDPB, [1,4-di-(2'-pyridyldithio propionamido) butane], in an attempt to stabilize a peptide-dependent dimeric structure. The choice of crosslinker was based on previous experiments with amine-reactive crosslinkers that were found to inactivate EBP. EBP contains a single free sulphydryl (Cys^{181}) in D2 which is potentially reactive to crosslinking reagents (The DPDPB crosslinker itself does not inactivate the EPO binding potential of EBP nor the proliferative properties of EMP1). A dimeric EBP product is formed by co-incubation of EMP1, DPDPB and EBP. The amount of dimeric product increases with peptide concentration and no significant dimer product is observed in the absence of peptide. DPDPB-crosslinked products formed through disulfide-exchange reactions should be readily reversible by reduction as is seen for the covalently-linked EMP1-mediated dimer. Furthermore, we have constructed a covalently-linked dimeric form of EMP1 that demonstrates increased biological potency (Johnson et al, in preparation). The Cys^{181} residues in D2 of the EBP dimer are 20.7 Å apart (Sγ-Sγ distance) which approximates the 16 Å length (and approximately 2 Å in bond length at each end) of the DPDPB cross-linker. Thus EMP1 mediates formation of a soluble EBP dimer complex in solution consistent with the crystal structure.

The WSXWS motif

The WSAWS sequence (residues 209-213) corresponding to the WSXWS box occurs in a β-bulge (Richardson, Adv. Prot. Chem. 34:167, 1981; Chan et al., Protein Science, 2:1574, 1993) immediately preceding β-strand G in D2. Residues in this motif do not interact with ligand, have no role in receptor-receptor interactions and are located on the opposite side of the receptor-receptor and receptor-ligand interface. The WSAWS box represents only a segment of a complex array of interactions that involves several other conserved side chains from the four-stranded β-sheet in D2. The indole ring systems of Trp^{209} and Trp^{212} point toward an external concave surface of the β-sheet and are only partially solvent exposed, whereas the Ala^{211} side chain points directly out into solution. The amides and hydroxyls of both Ser^{210} and Ser^{213} form hydrogen bonds with the main

chain of residues 198 and 196 of adjacent strand F in a pseudo β-sheet type interaction that resembles a modified wide β-bulge (Richardson, Adv. Prot. Chem. 34:167, 1981; Chan et al., Protein Science, 2:1574, 1993) where the sidechain hydroxyl rather than the carbonyl oxygen makes the β-sheet interaction. The β-bulge architecture places the two Trp residues, which are spread four residues apart, on the same side of the β-sheet and not on opposite sides as in normal β-sheet or extended chain structures. The guanidinum group of Arg^{197} from Strand F, the central residue (Richardson, Adv. Prot. Chem. 34: 167, 1981; Chan et al., Protein Science, 2:1574, 1993) in the bulge, is positioned exactly between the two Trp indole rings to form an extended π-cation system (Kumpf et al., Science 261:1708, 1993. The center of the pyrrole ring of Trp^{209}, the Nε of the Arg^{197} and the center of the benzene ring of Trp^{212} are positioned on a straight line with the three planes of the conjugated systems stacked parallel to each other at approximately 4 Å spacing. In addition, the aliphatic portion of the Arg^{199} side chain has hydrophobic interactions with the indole ring of Trp^{209}, completing the alternating stacking of two aromatic and two positively-charged amino acid residues. The side chain of Glu^{157} forms a hydrogen bond with Arg^{197} presumably to help orient the guanidinium group and add some specificity and stabilization to the system.

It appears then that the linear WSXWS motif identified from sequence alignments of cytokine receptors represents only a component of a more complex conformational unit that contributes a significant structural feature to D2. Aromatic residues have previously been suggested to have a stabilizing effect and play a role as a folding nuclei in structures of antiparallel β-sandwiches (Finkelstein et al., Protein Eng. 6:367, 1993). The amino-aromatic parallel stacking between the guanidinium group of arginine and the aromatic rings is a common feature in protein structures (Burley et al., Adv. Prot. Chem., 39:125, 1988; Flocco et al., J. Mol. Biol., 235:709, 1994), but a parallel triple stacking of π-cation systems is rare (Kim et al., Biochemistry 32:8465, 1993) although observed in other class-1 cytokine receptors, hGHbp and PRLR.

The structural equivalents of the WSXWS motif in hGHbp (YGEFS) and PRLR (WSAWS) are involved in an even more intricate and complex array of π-cation interactions. The π-cation system is extended in hGHbp and PRLR to include an additional aromatic residue (Trp^{186} for hGHbp and Trp^{156} for PRLR) from the loop region that links βC and βC' in D2 and a positively-charged residue (Arg^{211} for hGHbp and Arg^{147} for PRLR) that stacks between the Trp and the second aromatic residue. The additional Arg residue is contributed either from the βF strand as in hGHbp (Arg^{211}) or from βC as in PRLR (Arg^{147}); the glutamine residue that hydrogen bonds and orients the arginine also switches strands. Sequence alignments suggest that this Arg-Gln switch could be common to other members of the class-1 cytokine receptor family. The extended π-cation system in hGHbp and PRLR consists of five positively charged and three aromatic residues stacked in an alternating order which comprises of Lys^{215}, Tyr^{222}, Arg^{213}, Phe^{225}, Arg^{211}, Trp^{186}, Lys^{179} for hGHbp and Lys^{185}, Trp^{191}, Arg^{183}, Trp^{194}, Arg^{147}, Trp^{156}, Lys^{149} for PRLR. The first aromatic-Arg-aromatic trio are approximately 4Å apart, as in EBP, but the second system is stacked closer together at approximately 3.6 Å spacings consistent with π-π interaction (Burley et al., Adv. Prot. Chem., 39:125, 1988; Flocco et al., J. Mol. Biol., 235:709, 1994). The outer lysines also use the aliphatic portions of their side chains to form hydrophobic interactions with the aromatic rings. Based on sequence alignments with other members of the class-1 cytokine receptor superfamily, such structurally extended π-cation systems could exist in human thrombopietin, IL-6 and ciliary neurotrophic factor receptors, and in human IL-4 receptor based on structural modeling (Gustchina et al., Proteins 21:140, 1995). Although IFN-γRα and tissue factor do not have a WSXWS motif, the corresponding sequences TTEKS (residues 213-217) for IFN-γRα (Walter et al., Nature 376:230, 1995) and KSTDS (residues 201-205) for tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994), maintain a very similar β-bulge. The consensus sequence among these five x-ray structures indicates that a serine or threonine in positions 2 and 5 maintain a common set of hydrogen bonds between their side chain hydroxyls and the mainchain of the neighboring strand. Only in hGHbp is there no hydroxyl-containing residue in position 2, but Ser^{226} still maintains the equivalent interaction. A Ser^{226} to Ala

mutation abrogates hGHR binding to hGH, and its expression on the cell surface is drastically reduced (Baumgartner et al., J. Biol. Chem., 269: 29094, 1994). In GM-CSFRα and IL-2Rβ, point mutations of the serine residues cause a substantial decrease in cell surface expression but little or no effect on ligand binding (Ronco et al., J. Biol. Chem. 269:277, 1994; Miyazaki et al., EMBO Journal 10:3191, 1991).

Conservation of the WSXWS motif in EPOR or its equivalent in other members of the class 1 cytokine receptors has been proposed to be essential for biological activity and was thus assumed to be part of the receptor binding site (Yoshimura et al., J. Biol. Chem. 267:11619, 1992; Quelle, Mol. Cell. Biol. 12:4553 1992). For EPOR, a systematic study of 100 mutations of the WSAWS sequence demonstrates that most of the mutations of the two tryptophan and serine resulted in molecules that did not reach the cell surface but were retained in the endoplasmatic reticulum (Hilton et al., Proc. Natl. Acad. Sci. USA 92:190, 1995; Hilton et al., J. Biol. Chem. 271:4699, 1996). Furthermore, an Ala^{211} to Glu mutation in the WSAWS sequence resulted in better transportation from the ER to the Golgi and a 3-5 fold increase of the number of EPOR molecules on the cell surface compared to the wild-type (Hilton et al., Proc. Natl. Acad. Sci. USA 92:190, 1995; Hilton et al., J. Biol. Chem. 271:4699, 1996). These results support our conclusion that the WSXWS sequence plays an important role in the structure and folding of D2 in EPOR and other related receptors.

Comparison with other cytokine-receptor complex structures

The overall quaternary structure of the peptide-EBP complex substantially from the equivalent arrangement in the hGH-hGHR complex. The non-symmetric nature of the single four-helix-bundle structure of the growth hormone ligand results in an asymmetric homo-dimerization of the receptor that corresponds to a 159° rotation between receptors compared to the almost perfect 2-fold (180°) rotation for the EBP-peptide complex. The tertiary arrangement of domains within EBP and hGHbp is also somewhat different. When the equivalent EBP and hGHbp D2 domains are superimposed on each other, their corresponding D1 domains differ by a 12° rotation and a 4.3Å translati n.

The mechanism of hGH binding to its receptor has been well studied (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995) and is sequential. Initial high affinity (nM) binding of the hormone with one receptor results is a buried surface of 1130 Å^2 on the receptor. The second hGHbp2 has a substantially smaller interface (deVos et al., Science 255:306, 1992) with the second binding site on hGH and interacts only with the preformed 1:1 complex to generate buried surface areas of 740 Å^2 with hGH and 440 Å^2 with the first hGHbp1 (deVos et al., Science 255:306, 1992; (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995). The binding determinants of each hGHbp are comprised of the six recognition loops (L1-L6), three of which (L1-L3) come from one end of the β-sandwich structure in D1, one from the interdomain linker and two from D2.

Although these two receptor complexes, EBP-EMP1 and hGH-hGHbp, have different dimeric arrangements, which probably in this case represent differences in the size and shape of the natural versus synthetic ligand, both receptors share equivalent ligand recognition loops, L1, L3, L5 and L6 for the EBP and L1 to L6 for the hGHbp. A non-active PRLR, complexed with only one molecule of hGH, also uses the same contact loops (L1 to L6) (Somers et al., Nature 372:478, 1994). Based on similarity of the ligand recognition sites in hGHbp and PRLR, one would expect that the binding site of EBP, when its natural EPO ligand is bound, would extend to include two additional loops, L2 and L4, that comprise residues 59-63 (L2) between strands C to C', and residues 110-118 (L4) from the carboxyl end of βG in D1 and the interdomain linker. These six loops in EBP, hGHbp and PRLR area in structurally equivalent positions but vary in size, amino acid composition and conformation although the interacting portions of each loop (side or tip) remain similar; L1, L2, L3, L5 interact mainly with their tips and L6 with its side. In EBP, the L5 loop is three residues shorter than in hGHbp and PRLR, where the L6 loop is three and four residues longer than in hGHbp and PRLR, respectively. The L2 loop also varies (6 to 10 residues) among the three receptors but in EBP does not participate in peptide binding, and in hGHbp is partially disordered, although it does contact th hormone. In one respect, this situation is similar to the complementarity-

determining regions (CDR's) in antibodies, where changes in length and sequence of the six binding loops impose specificity for different antigens, whereas the framework itself remains constant (Wilson et al., Ciba Foundation Symposium. Wiley, Chichester, 1991, Vol. 159, p. 13).

It has been shown for the hGH-hGHbp complex that only a subset of 9 out of 33 interacting residues that make up the structural epitope of the receptor constitute a functional epitope or hot spot (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995) where high affinity binding interaction takes place. This reduced epitope is substantially smaller than the structural epitope and is comprised from residues (Arg^{43}, Glu^{44}, Ile^{103}, Trp^{104}, Ile^{105}, Pro^{106}, Asp^{165}, and Trp^{169}) which are located in contact loops L1, L3 and L5 with the most significant contribution (>4.5 kcal/mol) coming from two aromatic residues (Trp^{104} and Trp^{169}) in L3 and L5 (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Wells, Proc. Natl Acad. Sci. USA 93:1, 1996). In EBP, Phe^{93} is equivalent to Trp^{104} in hGHbp, as suggested previously (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Wells, Proc. Natl Acad. Sci. USA 93:1, 1996; Jolliffe et al., Nephrol. Dial. Trans. 10:suppl. 2, 28, 1995), but there is no homologous residue to Trp^{169} in the shorter L5 loop. In the EBP-EMP1 complex, the Phe^{P8} peptide aromatic side chain occupies the equivalent position of the Trp^{169} side chain in hGHbp. One can assume that when EPO binds to its receptor, the hormone may provide an aromatic residue to the hydrophobic core of the binding interface and/or the L6 loop in EBP may play a more significant role in the hormone binding than in hGHbp, since it is 3 residues longer and contains the aromatic Phe^{205}.

In these three class-1 receptor structures, some loops are disordered which are in D2 for EBP for EBP (residues 164-166 in EBP1 and 133-135 in EBP2) and in D1 for both hGHbp (residues 55-58, 73-78 for hGHbp1 and 54-60, 73-75 for hGHbp2) and PRLR (residues 31-33, 84-86). Otherwise, these three class-1 cytokine receptors do not differ greatly in their over all tertiary structures; D1 and D2 have broadly similar general

arrangement in all three receptors such that the angle between the long axes of the two domains is approximately 90 degrees. I tis this arrangement of domains that allow these particular L1-L6 loops to be available for the recognition and binding of ligands. In a 2:2 complex between IFN-γ and its class-2 receptor IFN-γRα, D1 and D2 are related by a 125 degree angle, which elongates the receptor and restricts the binding determinants that can be used for interaction with hormone; the L1 loop now becomes buried in the D1-D2 interface, although the other five loops (L2-L6) are still available for ligand interaction. This elongated interdomain arrangement is also observed in tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994) which has a distant relationship to the cytokine receptor superfamily.

A mutational analysis of the EBP molecule indicates that the most crucial amino acid residue for binding EPO is Phe^{93} in the L3 loop (Jolliffe et al., Nephrol. Dial. Trans. 10:suppl 2,28, 1995). The Phe93Ala mutant shows an increase int he IC_{50} compared to the wild-type by a factor of approximately 1000, whereas other mutants (Ser91Ala, Ser92Ala, Val94Ala, Met150Ala and His153Ala) show small relative increases in teh IC_{50} of only 2.5-12.5 fold). The side chain of Phe^{93} buries 66 $Å^2$ of molecular surface, which is the highest among interacting side chains. In hGHbp, the corresponding Trp104Ala mutation results in an increase in the K_d by a factor of more than 2,500 compared to the wild-type indicating the equivalent importance of this residue in hGH binding and its key contribution to the hydrophobic core of the functional epitope (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Bass et al. Proc. Natl. Acad. Sci. USA 88:4498, 1991).

The role of dimerization on signal transduction

In the EBP-EMP1 complex structure, we surprisingly observe that a peptide, unrelated in sequence and probably in structure, to the natural ligand, can induce a biologically active dimerization of EPO receptor that promotes signal transduction and cell proliferation. Comparison of three class-1 cytokine receptor complexes, whose structures hav been determined so far, suggests that when the natural EPO hormone, which is

proposed to have a structure of a four-helix bundle (Boissel et al., J. Biol. Chem. 268:15983, 1993), induces receptor dimerization, it is more likely to resemble the hGH-hGHbp assemblage. This would suggest that more than one mode of productive extracellular dimerization is permissive for intracellular dimerization of the cytoplasmic domains with two JAK2 molecules in order to initialize the cascade of events that produces the biologically relevant signal (Ihle et al., Seminars in Immunology 5:375, 1993; Klingmuller et al., Cell 80:729, 1995). The peptide-EBP structure would then represent only one possible dimeric arrangement that promotes signal transduction.

Mutant EPOR molecules, containing a single Arg to Cys mutation (Arg^{130} in human and Arg^{129} in murine), have been shown to form biologically active dimers in the absence of EPO (Yoshimura et al., J. Biol. Chem. 267:11619, 1992); Watowich et al., Proc. Natl. Acad. Sci. USA 89:2140, 1992; Watowich et al., Mol. Cell. Biol. 14:3535, 1994), suggesting that extracellular recptor homo-dimerization may be sufficient in itself for signal transduction. It has been shown in another system (Spencer et al., Science 262:1019, 1993) that activation of a specific set of trasncription factors can be induced by the chemical crosslinking of cytoplasmic domains of modified cell membrane receptors that do not contain the extracellular and transmembrane domains. These receptors are not related to the cytokine receptor superfamily but illustrate that oligomerication plays a key role in activation of the receptor, and that the main functional role of the extracellular, ligand-binding domain is to allow (in the presence of ligand) dimerization or oligomerization and induce similar association of the cytoplasmic domains.

Mutageneses experiments originally suggested a role for the WSXWS motif in this cell signalling process (Yoshimura et al., J. Biol. Chem. 267:11619, 1992; Quelle et al. Mol. Cell. Biol. 12:4553, 1992; Chiba et al., Biochem. Biophys. Res. Comm. 184:485, 1992) possibly by promoting receptor homo-dimerization. However, truncation mutants of EPOR (Miura et al., Arch. Biochem. Biophys. 306:200, 1993) do not confirm this role for the WSXWS motif. The EBP-EMP1 complex structure shows that the WSXWS motif

of the EPOR, as for the hGH-hGHbp complex (deVos et al., Science 255:306, 1992) is located on the opposite face of the molecule from the receptor dimerization. In the absence of unliganded structures for the extracellular domains of EPOR, hGHR and PRLR, it is not possible to determine whether any conformation change occurs on ligand binding that would involve the WSXWS box. Apart from being a striking structural feature in D2, and its obvious proximity to the membrane spanning domain, one cannot rule out possible interactions of this region with some other cell surface molecules that are involved somehow in the signal transduction process.

Towards design of small molecule mimetics

The structure of the EMP1 dimer demonstrates that a peptide considerably smaller than the natural hormone can act as an agonist and induce the appropriate biological response. The peptide can be assumed to form a substantially smaller contact interface than the natural hormone with the receptor. The peptide binding site in EBP forms an almost flat surface, which is mainly hydrophobic in nature, without any cavities or charged residues that are normally essential for the specific targeting of small molecule ligands to a receptor binding site. The hGHbp study (Wells et al., Science 267:383, 1995; Wells, Proc. Natl. Acad. Sci. USA 93:1, 1996) shows that only a small part of the observed structural binding site, the so-called functional epitope (supra), contributes most of the binding energy and strongly implied that a "minimized" hormone designed to interact with this site could form sufficient interactions to activate the receptor. Furthermore, the limited site of interaction of the small agonist peptide with the EBP corresponds almost exactly to the smaller functional epitope derived from alanine scanning of hGH and hGHbp. Thus, by a different approach, we have arrived at the similar conclusion that a small number of key interactions can contribute to a functional epitope on a receptor. Understanding of this simplified interaction surface can be now combined with further mutational studies to assist in identifying the most crucial residues in the functional epitope, and consequently provide a more practical target for drug design.

Data Collection, MIR and Refinement Statistics

The crystallographic data is summarized in Table 1. Native crystallographic data were collected on a Siemens multiwire area detector mounted on an Elliott GX-18 generator, operating at 40kV and 55mA, with a crystal-to-detector distance of 120mm. Two derivative data sets were collected on a MAR image plate mounted on a Siemens generator operating at 50kV and 80mA, with crystal-to-image plate distance of 150mm. Data were integrated, scaled and reduced using the programs XENGEN (Howard et al., J. App. Cryst. 20:383, 1987) for the native data and DENZO/SCALEPACK (Otwinowski et al., SERC Darsbury Laboratory, Warrington, 1993) for the derivative data. Initial multiple isomorphous replacement anomalous scattering (MIRAS) phases were calculated to 3.1 Å using the program package PHASES (Furey, American Crystallographic Association Fortieth Anniversary Meeting, New Orleans, LA, 1990) with a mean figure of merit of 0.64 (25.0-3.1 Å). Phases were refined in PHASES using the solvent flattening protocol to a mean figure of merit of 0.92 (25.0-3.1 Å). The quality of the map was generally good and most of the complex structure (94%) could be fitted using the graphics program O (Jone et al., Acta Crystallogr A47:110, 1991). The register of the amino acid residues was verified from the positions of the two disulfide bridges in D1, and the positions of the two Hg's from the mercury acetate derivative that were correctly assumed to bind to the free Cys^{181} residue. the peptide interpretation was verified from another data set from a complex between EBP and an iodinated peptide (Tyr^{P4} was substituted for *p*-iodo-Phe), which diffracted to 3.3Å resolution, that in difference Fourier $(F_{iodo}-F_{nat})\alpha_{MIRAS}$ gave a clear indication of the location of the iodine atoms. The structure was refined using the slow-cooling protocol in X-PLOR 3.1(Brunger et al., Acta Crystallogr. A46:585, 1990; Brunger, X-PLOR, Version 3.1: A System for X-ray and NMR, Yale Univ. Press, New Haven, CT, 1992) and rebuilt using Fo-Fc, 3Fo-2Fc and SIGMAA(Read, Acta Crystallogr. A42:140, 1986) weighted electron density maps. After every two cycles of refinement, a set of simulated annealing omit maps (7-10%) to reduce model bias was calculated and the entire structure rebuilt. After several cycles of refinement, individual temperature factors were calculated and after 10 cycles of refinement and model building, the R-value was 0.21 for 8.0-2.8 Å data with $F>1\sigma$ (13,984 reflections). The average thermal parameters for receptor I, receptor II and the

peptides are 10.5Å^2, 12.3Å and 10.7Å respectively. Only one non-glycine residue [Asn^{164} in EBP2], located in a loop region in D1, is in a disallowed region in the Ramachandran plot. No solvent molecules were included in the model due to the moderate resolution (2.8 Å) of the structure determination.

Binding Contacts

Binding contacts are summarized, in part, in Table 2: Hydrogen bond interactions in the binding site of the EBP-EMP1 complex. Due to the symmetrical nature of the complex, peptide-1 and peptide-2 have equivalent interactions with the two EBP molecules. The hydrogen bond interactions were analyzed using HBPLUS (McDonald et al., J. Mol. Biol. 238:777, 1994), based upon both distance (3.9 Å cutoff) and geometrical considerations.

A number of embodiments of the present invention have been described. Nevertheless, it will be understood that various modifications may be made without departing from the spirit and scope of the invention. Accordingly, it is to be understood that the invention is not to be limited by the specific illustrated embodiment, but only by the scope of the appended claims.

all.con Thu Apr 25 15:08:07 1996 1

EBP1-PEPTIDE1

VDW	1	LEU	33	CB	4	PHE	308	CE1	1	3.95
VDW	1	LEU	33	CB	4	PHE	308	CD1	1	4.11
VDW	1	PHE	93	CE1	4	TRP	313	CH2	1	3.74
VDW	1	PHE	93	CZ	4	TRP	313	CH2	1	3.98
VDW	1	PHE	93	CZ	4	TRP	313	CZ2	1	4.08
VDW	1	PRO	149	CA	4	GLY	309	O	1	3.59
VDW	1	PRO	149	CB	4	GLY	309	O	1	3.49
VDW	1	PRO	149	C	4	GLY	309	O	1	3.66
VDW	1	MET	150	N	4	PRO	310	O	1	3.35
VDW	1	MET	150	N	4	PRO	310	C	1	3.62
VDW	1	MET	150	CA	4	LEU	311	O	1	3.41
VDW	1	MET	150	CA	4	GLY	309	O	1	3.78
VDW	1	MET	150	CA	4	LEU	311	C	1	3.87
VDW	1	MET	150	CG	4	PHE	308	CD2	1	3.50
VDW	1	MET	150	CG	4	PHE	308	CB	1	3.70
VDW	1	MET	150	CG	4	PHE	308	CG	1	3.79
VDW	1	MET	150	SD	4	PHE	308	CD2	1	3.52
VDW	1	MET	150	SD	4	THR	312	C	1	3.55
VDW	1	MET	150	SD	4	THR	312	CA	1	3.58
VDW	1	MET	150	SD	4	TRP	313	N	1	3.75
VDW	1	MET	150	SD	4	PHE	308	CA	1	3.91
VDW	1	MET	150	SD	4	PHE	308	CB	1	4.03
VDW	1	MET	150	CE	4	PHE	308	CD2	1	3.45
VDW	1	MET	150	CE	4	TRP	313	CE2	1	3.71
VDW	1	MET	150	CE	4	PHE	308	CE2	1	3.79
VDW	1	MET	150	CE	4	TRP	313	CD2	1	3.83
VDW	1	MET	150	CE	4	TRP	313	NE1	1	3.91
VDW	1	MET	150	CE	4	TRP	313	CZ2	1	4.10
VDW	1	MET	150	C	4	LEU	311	O	1	3.41
VDW	1	THR	151	N	4	LEU	311	O	1	3.45
VDW	1	THR	151	CA	4	PRO	310	O	1	3.82
VDW	1	THR	151	CB	4	PRO	310	O	1	3.56
VDW	1	THR	151	OG1	4	LEU	311	CD2	1	3.43
VDW	1	THR	151	OG1	4	LEU	311	CA	1	3.91
VDW	1	THR	151	CG2	4	PRO	310	O	1	3.60
VDW	1	SER	152	CB	4	LEU	311	O	1	3.54
VDW	1	HIS	153	ND1	4	LEU	311	O	1	3.57
SHORTVDW	1	HIS	153	CE1	4	THR	312	OG1	1	2.87
VDW	1	HIS	153	CE1	4	THR	312	CB	1	3.48
VDW	1	HIS	153	CE1	4	THR	312	CA	1	3.76
VDW	1	HIS	153	NE2	4	THR	312	OG1	1	3.57
VDW	1	PHE	205	CE2	4	PHE	308	CZ	1	3.90
VDW	1	PHE	205	CZ	4	PHE	308	CE2	1	3.40
VDW	1	PHE	205	CZ	4	PHE	308	CZ	1	3.53

EBP2-PEP1

VDW	2	SER	591	CA	4	TYR	304	OH	1	3.44
VDW	2	SER	591	CB	4	TYR	304	OH	1	3.88
VDW	2	SER	591	CB	4	PRO	317	CB	1	3.95
VDW	2	SER	591	OG	4	TYR	304	OH	1	3.44
VDW	2	SER	591	OG	4	PRO	317	CB	1	3.61
VDW	2	SER	591	OG	4	TYR	304	CZ	1	3.83
VDW	2	SER	591	OG	4	TYR	304	CE2	1	3.84
VDW	2	SER	591	C	4	TYR	304	OH	1	3.62
VDW	2	SER	592	N	4	TYR	304	CE2	1	3.66
VDW	2	SER	592	N	4	TYR	304	CZ	1	3.68
VDW	2	SER	592	CA	4	TYR	304	OH	1	3.80
VDW	2	SER	592	CB	4	TYR	304	OH	1	3.73
VDW	2	SER	592	C	4	TYR	304	CE2	1	4.00
VDW	2	SER	592	O	4	TYR	304	CE2	1	3.53
VDW	2	SER	592	O	4	PRO	317	CD	1	3.59
VDW	2	PHE	593	CB	4	CYS	315	O	1	3.74
VDW	2	PHE	593	CD1	4	CYS	315	CB	1	3.55
VDW	2	PHE	593	CD1	4	TYR	304	CD2	1	3.72

all.con Thu Apr 25 15:08:07 1996 2

VDW	2	PHE	593	CD1	4	TYR	304	CE2	1	3.90
VDW	2	PHE	593	CE1	4	CYS	315	CB	1	3.71
SHORTVDW	2	VAL	594	CG1	4	PRO	317	CG	1	3.17
SHORTVDW	2	VAL	594	CG1	4	PRO	317	CD	1	3.23
EBP1-PEPTIDE2										
VDW	1	SER	91	CB	4	PRO	417	CB	1	3.84
VDW	1	SER	91	CB	4	PRO	417	CG	1	3.90
VDW	1	SER	91	OG	4	PRO	417	CB	1	3.90
VDW	1	SER	92	N	4	TYR	404	CE2	1	3.82
VDW	1	SER	92	CA	4	TYR	404	OH	1	3.85
VDW	1	SER	92	CB	4	TYR	404	OH	1	3.42
VDW	1	SER	92	CB	4	TYR	404	CZ	1	4.04
VDW	1	SER	92	CB	4	TYR	404	CE2	1	4.09
VDW	1	PHE	93	CB	4	CYS	415	O	1	3.43
VDW	1	PHE	93	CD1	4	TYR	404	CE2	1	3.71
VDW	1	PHE	93	CD1	4	TYR	404	CD2	1	3.83
VDW	1	PHE	93	CD1	4	CYS	415	CB	1	3.92
VDW	1	PHE	93	CE1	4	CYS	415	CB	1	4.08
VDW	1	PHE	93	CE1	4	TYR	404	CE2	1	4.09
VDW	1	VAL	94	CG1	4	PRO	417	CG	1	3.54
VDW	1	VAL	94	CG1	4	PRO	417	CD	1	3.54
VDW	1	VAL	94	CG2	4	PRO	417	CG	1	4.11
EBP2-PEPTIDE2										
SHORTVDW	2	LEU	533	CB	4	PHE	408	CE1	1	3.14
VDW	2	LEU	533	CB	4	PHE	408	CD1	1	3.77
VDW	2	LEU	533	CB	4	PHE	408	CZ	1	4.00
VDW	2	LEU	533	CG	4	PHE	408	CE1	1	4.05
VDW	2	LEU	533	CD1	4	PHE	408	CE1	1	3.75
VDW	2	LEU	533	CD1	4	PHE	408	CZ	1	3.92
VDW	2	LEU	533	O	4	PHE	408	CE1	1	3.67
VDW	2	PHE	593	CE1	4	TRP	413	CH2	1	3.34
VDW	2	PHE	593	CE1	4	TRP	413	CZ2	1	3.41
VDW	2	PHE	593	CZ	4	TRP	413	CZ2	1	3.67
VDW	2	PHE	593	CZ	4	TRP	413	CH2	1	3.96
VDW	2	PRO	649	CA	4	GLY	409	O	1	3.79
VDW	2	PRO	649	CB	4	GLY	409	O	1	3.56
VDW	2	PRO	649	C	4	PRO	410	O	1	3.72
VDW	2	MET	650	CA	4	PRO	410	O	1	3.59
VDW	2	MET	650	CA	4	GLY	409	O	1	3.67
VDW	2	MET	650	CA	4	LEU	411	O	1	3.77
VDW	2	MET	650	CG	4	PHE	408	CD2	1	3.80
VDW	2	MET	650	CG	4	PHE	408	CG	1	3.92
VDW	2	MET	650	CG	4	PHE	408	CB	1	4.05
VDW	2	MET	650	SD	4	TRP	413	N	1	3.72
VDW	2	MET	650	SD	4	THR	412	C	1	3.75
VDW	2	MET	650	SD	4	PHE	408	CD2	1	3.76
VDW	2	MET	650	SD	4	THR	412	CA	1	3.78
VDW	2	MET	650	SD	4	PHE	408	CA	1	4.02
VDW	2	MET	650	CE	4	TRP	413	CE2	1	3.67
VDW	2	MET	650	CE	4	TRP	413	NE1	1	3.76
VDW	2	MET	650	CE	4	TRP	413	CD2	1	3.76
VDW	2	MET	650	CE	4	PHE	408	CD2	1	3.83
VDW	2	MET	650	CE	4	TRP	413	CD1	1	3.88
VDW	2	MET	650	CE	4	TRP	413	N	1	3.89
VDW	2	MET	650	CE	4	TRP	413	CG	1	3.90
VDW	2	MET	650	C	4	LEU	411	O	1	3.54
VDW	2	MET	650	C	4	PRO	410	O	1	3.57
VDW	2	THR	651	N	4	LEU	411	O	1	3.56
VDW	2	THR	651	N	4	PRO	410	C	1	3.77
VDW	2	THR	651	CA	4	PRO	410	O	1	3.41
SHORTVDW	2	THR	651	CB	4	PRO	410	O	1	3.03
VDW	2	THR	651	CB	4	PRO	410	C	1	3.98
VDW	2	THR	651	CB	4	LEU	411	CA	1	4.02
VDW	2	THR	651	OG1	4	PRO	410	C	1	3.62

all.con Thu Apr 25 15:08:07 1996 3

VDW	2	SER	652	N	4	LEU	411	C	1	3.83
VDW	2	SER	652	CA	4	LEU	411	O	1	3.51
VDW	2	SER	652	CB	4	LEU	411	O	1	3.18
VDW	2	SER	652	CB	4	LEU	411	C	1	4.09
VDW	2	SER	652	OG	4	THR	412	CB	1	3.73
SHORTVDW	2	HIS	653	CE1	4	THR	412	OG1	1	3.00
VDW	2	HIS	653	CE1	4	THR	412	CB	1	3.91
PEPTIDE1-PEPTIDE2										
SHORTVDW	3	THR	303	OG1	4	HIS	407	CB	1	2.94
VDW	3	THR	303	OG1	4	HIS	407	CA	1	3.61
VDW	3	TYR	304	CB	4	CYS	406	O	1	3.86
VDW	3	TYR	304	CD1	4	TRP	413	CZ3	1	3.81
VDW	3	TYR	304	CD1	4	TRP	413	CH2	1	3.94
VDW	3	TYR	304	O	4	CYS	406	N	1	3.33
VDW	3	TYR	304	O	4	CYS	406	O	1	3.47
VDW	3	TYR	304	O	4	SER	405	CA	1	3.57
VDW	3	SER	305	CA	4	TYR	404	O	1	3.51
VDW	3	SER	305	C	4	TYR	404	O	1	3.77
VDW	3	CYS	306	O	4	THR	403	CB	1	3.50
VDW	3	CYS	306	O	4	TYR	404	CB	1	3.54
VDW	3	CYS	306	O	4	TYR	404	CD1	1	3.59
VDW	3	CYS	306	O	4	TYR	404	CA	1	3.75
VDW	3	CYS	306	CB	4	CYS	406	SG	1	3.81
VDW	3	CYS	306	SG	4	CYS	406	SG	1	3.75
VDW	3	CYS	306	SG	4	CYS	406	CB	1	4.06
VDW	3	PHE	308	CE1	4	TYR	404	OH	1	3.93
VDW	3	PHE	308	CE1	4	TYR	404	CE1	1	4.08
VDW	3	TRP	313	CG	4	TRP	413	CD1	1	3.85
SHORTVDW	3	TRP	313	CD1	4	TRP	413	CD1	1	3.04
VDW	3	TRP	313	CD1	4	TRP	413	NE1	1	3.37
VDW	3	TRP	313	CD1	4	TRP	413	CG	1	4.09
VDW	3	TRP	313	NE1	4	TRP	413	CD1	1	3.31
VDW	3	TRP	313	CZ2	4	CYS	415	SG	1	3.84
VDW	3	TRP	313	CH2	4	CYS	415	SG	1	3.83
VDW	3	CYS	315	SG	4	TRP	413	CZ2	1	3.59
VDW	3	CYS	315	SG	4	TRP	413	CE2	1	3.95
VDW	3	CYS	315	SG	4	TRP	413	CH2	1	4.00
VDW	3	GLN	318	CD	4	GLN	418	NE2	1	3.28
VDW	3	GLN	318	OE1	4	SER	405	CB	1	3.80

bref21c.pdb Thu Apr 25 12:27:47 1996 1

```
REMARK  THE COMPLEX BETWEEN THE EXTRACELLULAR DOMAIN OF ERYTHROPOIETIN
REMARK  RECEPTOR (EBP) AND AN AGONIST EPO MIMETIC PEPTIDE 1 (EMP1)
REMARK  ***** WARNING **** RESIDUES 21-23 (521-523) and 164-166, 633-635
REMARK  HAVE WEAK OR NO ELECTRON DENSITY MAP AND HAVE BEEN MODELED
REMARK  INTO THE STRUCTURE.  THESE RESIDUES HAVE A HIGH B OF 99.
REMARK
REMARK  THE STRUCTURE CONSISTS OF TWO RECEPTOR (RESIDUES 10-220, 510-720)
REMARK  AND PEPTIDE (RESIDUES 303-318, 403 418) MOLECULES.
ATOM      1  N   LYS    10      40.090  29.257  22.042  1.00 22.57
ATOM      2  CA  LYS    10      39.634  30.133  20.962  1.00 23.45
ATOM      3  CB  LYS    10      38.753  29.361  19.979  1.00 22.87
ATOM      4  CG  LYS    10      38.334  30.155  18.735  1.00 22.92
ATOM      5  CD  LYS    10      38.119  29.212  17.552  1.00 24.27
ATOM      6  CE  LYS    10      37.165  28.015  17.890  1.00 26.55
ATOM      7  NZ  LYS    10      35.685  28.367  17.998  1.00 26.18
ATOM      8  C   LYS    10      38.921  31.427  21.420  1.00 22.91
ATOM      9  O   LYS    10      39.589  32.442  21.636  1.00 24.17
ATOM     10  N   PHE    11      37.602  31.386  21.640  1.00 21.40
ATOM     11  CA  PHE    11      36.868  32.588  22.026  1.00 18.56
ATOM     12  CB  PHE    11      35.549  32.257  22.725  1.00 19.07
ATOM     13  CG  PHE    11      34.497  33.362  22.609  1.00 20.24
ATOM     14  CD1 PHE    11      34.862  34.717  22.670  1.00 19.49
ATOM     15  CD2 PHE    11      33.142  33.038  22.400  1.00 19.51
ATOM     16  CE1 PHE    11      33.910  35.728  22.527  1.00 19.64
ATOM     17  CE2 PHE    11      32.180  34.041  22.257  1.00 20.10
ATOM     18  CZ  PHE    11      32.566  35.395  22.321  1.00 19.48
ATOM     19  C   PHE    11      31.644  33.567  22.887  1.00 19.32
ATOM     20  O   PHE    11      37.778  34.740  22.516  1.00 18.89
ATOM     21  N   GLU    12      38.181  33.106  24.016  1.00 20.71
ATOM     22  CA  GLU    12      38.905  34.036  24.886  1.00 20.59
ATOM     23  CB  GLU    12      39.253  33.423  26.246  1.00 21.48
ATOM     24  CG  GLU    12      40.185  34.309  27.123  1.00 23.60
ATOM     25  CD  GLU    12      39.455  35.301  28.056  1.00 25.09
ATOM     26  OE1 GLU    12      40.024  36.417  28.275  1.00 23.07
ATOM     27  OE2 GLU    12      38.356  34.952  28.589  1.00 21.05
ATOM     28  C   GLU    12      40.137  34.539  24.172  1.00 19.22
ATOM     29  O   GLU    12      40.513  35.703  24.334  1.00 18.49
ATOM     30  N   SER    13      40.730  33.687  23.341  1.00 17.67
ATOM     31  CA  SER    13      41.903  34.094  22.571  1.00 16.71
ATOM     32  CB  SER    13      42.522  32.898  21.851  1.00 18.51
ATOM     33  OG  SER    13      42.256  32.959  20.459  1.00 23.19
ATOM     34  C   SER    13      41.570  35.202  21.554  1.00 15.57
ATOM     35  O   SER    13      42.239  36.248  21.546  1.00 15.13
ATOM     36  N   LYS    14      40.562  34.955  20.698  1.00 12.00
ATOM     37  CA  LYS    14      40.117  35.912  19.675  1.00  8.51
ATOM     38  CB  LYS    14      39.063  35.287  18.769  1.00  5.06
ATOM     39  CG  LYS    14      39.629  34.366  17.714  1.00  2.36
ATOM     40  CD  LYS    14      38.566  33.862  16.761  1.00  2.00
ATOM     41  CE  LYS    14      39.191  33.270  15.496  1.00  2.27
ATOM     42  NZ  LYS    14      38.193  32.742  14.528  1.00  2.00
ATOM     43  C   LYS    14      39.586  37.198  20.295  1.00  9.05
ATOM     44  O   LYS    14      39.782  38.290  19.755  1.00  7.15
ATOM     45  N   ALA    15      38.920  37.053  21.442  1.00 11.98
ATOM     46  CA  ALA    15      38.375  38.188  22.194  1.00 12.13
ATOM     47  CB  ALA    15      37.571  37.697  23.378  1.00 11.49
ATOM     48  C   ALA    15      39.592  38.960  22.666  1.00 12.49
ATOM     49  O   ALA    15      39.683  40.189  22.535  1.00 13.58
ATOM     50  N   ALA    16      40.560  38.207  23.167  1.00 13.97
ATOM     51  CA  ALA    16      41.792  38.796  23.615  1.00 14.97
ATOM     52  CB  ALA    16      42.771  37.719  24.052  1.00 14.76
ATOM     53  C   ALA    16      42.361  39.567  22.426  1.00 15.45
ATOM     54  O   ALA    16      42.624  40.759  22.537  1.00 15.85
ATOM     55  N   LEU    17      42.444  38.896  21.274  1.00 16.12
ATOM     56  CA  LEU    17      43.007  39.467  20.042  1.00 15.92
ATOM     57  CB  LEU    17      43.013  38.428  18.910  1.00 15.72
ATOM     58  CG  LEU    17      44.204  37.485  18.662  1.00 17.46
ATOM     59  CD1 LEU    17      45.474  38.294  18.506  1.00 16.45
ATOM     60  CD2 LEU    17      44.360  36.462  19.774  1.00 16.32
ATOM     61  C   LEU    17      42.374  40.741  19.512  1.00 15.04
ATOM     62  O   LEU    17      42.985  41.438  18.711  1.00 15.91
ATOM     63  N   LEU    18      41.136  41.018  19.908  1.00 17.04
ATOM     64  CA  LEU    18      40.434  42.210  19.443  1.00 15.72
ATOM     65  CB  LEU    18      38.999  41.867  19.022  1.00 13.72
ATOM     66  CG  LEU    18      38.725  41.263  17.640  1.00  9.76
ATOM     67  CD1 LEU    18      37.235  41.260  17.329  1.00  5.61
ATOM     68  CD2 LEU    18      39.422  42.117  16.625  1.00 10.13
ATOM     69  C   LEU    18      40.393  43.284  20.500  1.00 17.38
ATOM     70  O   LEU    18      39.876  44.375  20.257  1.00 19.32
```

bref21c.pdb Thu Apr 25 12:27:47 1996 2

```
ATOM     71  N   ALA  19      40.921  42.981  21.680  1.00 19.88      7
ATOM     72  CA  ALA  19      40.925  43.941  22.789  1.00 22.64      6
ATOM     73  CB  ALA  19      41.560  43.331  24.041  1.00 22.75      6
ATOM     74  C   ALA  19      41.601  45.273  22.445  1.00 25.13      6
ATOM     75  O   ALA  19      42.026  45.499  21.294  1.00 25.03      8
ATOM     76  N   ALA  20      41.649  46.164  23.453  1.00 28.77      7
ATOM     77  CA  ALA  20      42.246  47.514  23.333  1.00 28.51      6
ATOM     78  CB  ALA  20      41.529  48.505  24.310  1.00 28.93      6
ATOM     79  C   ALA  20      43.770  47.526  23.562  1.00 27.54      6
ATOM     80  O   ALA  20      44.438  46.484  23.505  1.00 27.85      8
ATOM     81  N   ARG  21      44.326  48.699  23.848  1.00 90.00      7
ATOM     82  CA  ARG  21      45.765  48.784  24.075  1.00 90.00      6
ATOM     83  CB  ARG  21      46.562  48.353  22.819  1.00 90.00      6
ATOM     84  CG  ARG  21      45.827  48.428  21.446  1.00 90.00      6
ATOM     85  CD  ARG  21      45.719  49.838  20.863  1.00 90.00      6
ATOM     86  NE  ARG  21      44.765  50.675  21.591  1.00 90.00      7
ATOM     87  CZ  ARG  21      43.448  50.471  21.610  1.00 90.00      6
ATOM     88  NH1 ARG  21      42.915  49.448  20.926  1.00 90.00      7
ATOM     89  NH2 ARG  21      42.669  51.270  22.350  1.00 90.00      7
ATOM     90  C   ARG  21      46.298  50.118  24.590  1.00 90.00      6
ATOM     91  O   ARG  21      45.875  51.199  24.132  1.00 90.00      8
ATOM     92  N   GLY  22      47.158  50.016  25.614  1.00 90.00      7
ATOM     93  CA  GLY  22      47.824  51.171  26.193  1.00 90.00      6
ATOM     94  C   GLY  22      49.052  51.371  25.314  1.00 90.00      6
ATOM     95  O   GLY  22      48.939  51.174  24.089  1.00 90.00      8
ATOM     96  N   PRO  23      50.230  51.765  25.872  1.00 90.00      7
ATOM     97  CD  PRO  23      50.316  52.564  27.119  1.00 90.00      6
ATOM     98  CA  PRO  23      51.451  51.971  25.062  1.00 90.00      6
ATOM     99  CB  PRO  23      51.713  53.452  25.287  1.00 90.00      6
ATOM    100  CG  PRO  23      51.527  53.517  26.850  1.00 90.00      6
ATOM    101  C   PRO  23      52.681  51.167  25.544  1.00 90.00      6
ATOM    102  O   PRO  23      52.560  50.067  26.123  1.00 90.00      8
ATOM    103  N   GLU  24      53.863  51.758  25.368  1.00 28.27      7
ATOM    104  CA  GLU  24      55.136  51.178  25.741  1.00 24.32      6
ATOM    105  CB  GLU  24      56.332  52.009  25.238  1.00 24.01      6
ATOM    106  CG  GLU  24      56.479  52.149  23.723  1.00 25.03      6
ATOM    107  CD  GLU  24      56.710  50.822  22.959  1.00 24.22      6
ATOM    108  OE1 GLU  24      57.171  50.954  21.793  1.00 23.14      8
ATOM    109  OE2 GLU  24      56.430  49.692  23.478  1.00 18.50      8
ATOM    110  C   GLU  24      55.117  51.264  27.268  1.00 23.39      6
ATOM    111  O   GLU  24      54.874  52.365  27.829  1.00 24.36      8
ATOM    112  N   GLU  25      55.342  50.124  27.925  1.00 18.35      7
ATOM    113  CA  GLU  25      55.371  50.058  29.377  1.00 14.09      6
ATOM    114  CB  GLU  25      53.962  49.818  29.907  1.00 17.09      6
ATOM    115  CG  GLU  25      53.789  49.985  31.410  1.00 22.21      6
ATOM    116  CD  GLU  25      53.199  51.348  31.799  1.00 27.17      6
ATOM    117  OE1 GLU  25      53.461  52.355  31.057  1.00 27.15      8
ATOM    118  OE2 GLU  25      52.461  51.401  32.827  1.00 26.11      8
ATOM    119  C   GLU  25      56.249  48.872  29.725  1.00 11.99      6
ATOM    120  O   GLU  25      56.056  47.779  29.181  1.00 14.38      8
ATOM    121  N   LEU  26      57.246  49.098  30.572  1.00  8.48      7
ATOM    122  CA  LEU  26      58.147  48.034  31.001  1.00  5.93      6
ATOM    123  CB  LEU  26      59.398  48.624  31.652  1.00  4.03      6
ATOM    124  CG  LEU  26      60.719  47.880  31.488  1.00  2.00      6
ATOM    125  CD1 LEU  26      61.537  48.145  32.764  1.00  4.41      6
ATOM    126  CD2 LEU  26      60.535  46.401  31.317  1.00  2.00      6
ATOM    127  C   LEU  26      57.409  47.188  32.030  1.00  6.68      6
ATOM    128  O   LEU  26      56.951  47.727  33.041  1.00  9.43      8
ATOM    129  N   LEU  27      57.310  45.880  31.797  1.00  5.17      7
ATOM    130  CA  LEU  27      56.612  44.996  32.719  1.00  5.71      6
ATOM    131  CB  LEU  27      55.426  44.334  32.035  1.00  6.50      6
ATOM    132  CG  LEU  27      54.281  45.268  31.673  1.00 10.84      6
ATOM    133  CD1 LEU  27      53.101  44.428  31.125  1.00 10.81      6
ATOM    134  CD2 LEU  27      53.871  46.133  32.906  1.00  7.98      6
ATOM    135  C   LEU  27      57.454  43.923  33.397  1.00  7.41      6
ATOM    136  O   LEU  27      58.002  43.037  32.742  1.00  7.62      8
ATOM    137  N   CYS  28      57.460  43.964  34.726  1.00  7.42      7
ATOM    138  CA  CYS  28      58.208  43.027  35.554  1.00  4.67      6
ATOM    139  C   CYS  28      57.246  42.359  36.529  1.00  4.38      6
ATOM    140  O   CYS  28      56.217  42.945  36.861  1.00  2.56      8
ATOM    141  CB  CYS  28      59.266  43.791  36.357  1.00  3.64      6
ATOM    142  SG  CYS  28      60.429  44.763  35.358  1.00  4.87     16
ATOM    143  N   PHE  29      57.595  41.153  36.977  1.00  2.00      7
ATOM    144  CA  PHE  29      56.817  40.403  37.943  1.00  2.00      6
ATOM    145  CB  PHE  29      55.474  39.899  37.322  1.00  4.36      6
ATOM    146  CG  PHE  29      55.586  38.643  36.427  1.00  3.43      6
ATOM    147  CD1 PHE  29      55.493  37.369  36.990  1.00  2.00      6
ATOM    148  CD2 PHE  29      55.790  38.747  35.058  1.00  2.00      6
```

bref21c.pdb Thu Apr 25 12:27:47 1996 3

ATOM	149	CE1	PHE	29	55.605	36.243	26.206	1.00	2.00	S
ATOM	150	CE2	PHE	29	55.906	37.616	24.266	1.00	2.00	S
ATOM	151	CZ	PHE	29	55.815	36.365	24.843	1.00	2.00	S
ATOM	152	C	PHE	29	57.678	39.260	28.543	1.00	3.80	S
ATOM	153	O	PHE	29	58.702	38.897	27.957	1.00	2.00	S
ATOM	154	N	THR	30	57.340	38.814	29.766	1.00	4.17	7
ATOM	155	CA	THR	30	58.021	37.694	30.463	1.00	3.12	S
ATOM	156	CB	THR	30	58.720	38.116	31.820	1.00	2.00	S
ATOM	157	OG1	THR	30	59.337	36.982	32.408	1.00	2.00	S
ATOM	158	CG2	THR	30	57.763	36.661	32.827	1.00	2.00	S
ATOM	159	C	THR	30	56.951	36.601	30.674	1.00	6.81	S
ATOM	160	O	THR	30	55.774	36.924	30.814	1.00	8.70	S
ATOM	161	N	GLU	31	57.342	35.326	30.665	1.00	7.95	7
ATOM	162	CA	GLU	31	56.378	34.219	30.786	1.00	8.18	S
ATOM	163	CB	GLU	31	56.577	33.240	29.650	1.00	7.89	S
ATOM	164	CG	GLU	31	56.490	33.821	28.286	1.00	8.99	S
ATOM	165	CD	GLU	31	56.651	32.750	27.248	1.00	10.58	S
ATOM	166	OE1	GLU	31	57.538	32.875	26.395	1.00	13.03	S
ATOM	167	OE2	GLU	31	55.916	31.753	27.302	1.00	14.01	S
ATOM	168	C	GLU	31	56.453	32.432	32.079	1.00	8.38	S
ATOM	169	O	GLU	31	55.437	32.940	32.582	1.00	9.78	S
ATOM	170	N	ARG	32	57.678	33.064	32.416	1.00	7.19	7
ATOM	171	CA	ARG	32	58.006	32.390	33.670	1.00	8.64	S
ATOM	172	CB	ARG	32	58.844	31.154	33.405	1.00	9.16	S
ATOM	173	CG	ARG	32	58.284	30.364	32.261	1.00	10.75	S
ATOM	174	CD	ARG	32	58.376	28.894	32.469	1.00	11.21	S
ATOM	175	NE	ARG	32	57.070	28.271	32.295	1.00	13.52	7
ATOM	176	CZ	ARG	32	56.326	28.350	31.187	1.00	16.55	S
ATOM	177	NH1	ARG	32	56.763	29.036	30.128	1.00	17.12	7
ATOM	178	NH2	ARG	32	55.145	27.734	31.128	1.00	17.67	7
ATOM	179	C	ARG	32	58.834	32.536	34.224	1.00	9.21	S
ATOM	180	O	ARG	32	59.004	34.526	33.520	1.00	13.37	S
ATOM	181	N	LEU	33	59.382	33.499	35.416	1.00	7.72	7
ATOM	182	CA	LEU	33	60.084	34.736	35.716	1.00	8.01	S
ATOM	183	CB	LEU	33	59.536	35.403	36.986	1.00	7.85	S
ATOM	184	CG	LEU	33	58.323	36.310	36.699	1.00	2.00	S
ATOM	185	CD1	LEU	33	57.061	35.584	37.032	1.00	3.91	S
ATOM	186	CD2	LEU	33	58.381	37.604	37.464	1.00	2.00	S
ATOM	187	C	LEU	33	61.610	34.893	35.506	1.00	8.52	S
ATOM	188	O	LEU	33	62.269	35.702	36.168	1.00	10.67	S
ATOM	189	N	GLU	34	62.130	34.174	34.516	1.00	6.25	7
ATOM	190	CA	GLU	34	63.339	34.210	34.144	1.00	8.09	S
ATOM	191	CB	GLU	34	64.315	33.005	34.733	1.00	10.89	S
ATOM	192	CG	GLU	34	63.518	31.931	35.547	1.00	18.21	S
ATOM	193	CD	GLU	34	62.754	30.858	34.699	1.00	21.61	S
ATOM	194	OE1	GLU	34	61.810	30.224	35.257	1.00	22.26	S
ATOM	195	OE2	GLU	34	63.082	30.645	33.494	1.00	22.29	S
ATOM	196	C	GLU	34	62.678	34.239	32.594	1.00	7.89	S
ATOM	197	O	GLU	34	64.413	33.459	32.016	1.00	10.91	S
ATOM	198	N	ASP	35	62.978	35.150	31.933	1.00	6.40	7
ATOM	199	CA	ASP	35	62.981	35.244	30.483	1.00	4.88	S
ATOM	200	CB	ASP	35	62.215	34.034	29.895	1.00	5.00	S
ATOM	201	CG	ASP	35	60.678	34.189	29.957	1.00	6.69	S
ATOM	202	OD1	ASP	35	60.055	34.542	28.912	1.00	6.86	S
ATOM	203	OD2	ASP	35	60.102	33.911	31.025	1.00	2.00	S
ATOM	204	C	ASP	35	62.236	36.566	30.016	1.00	3.42	S
ATOM	205	O	ASP	35	61.562	37.153	30.731	1.00	4.41	S
ATOM	206	N	LEU	36	62.677	37.046	29.834	1.00	2.00	7
ATOM	207	CA	LEU	36	62.098	38.272	29.317	1.00	2.00	S
ATOM	208	CB	LEU	36	62.902	39.484	28.745	1.00	2.00	S
ATOM	209	CG	LEU	36	62.219	40.825	28.490	1.00	2.40	S
ATOM	210	CD1	LEU	36	60.994	40.997	29.365	1.00	2.31	S
ATOM	211	CD2	LEU	36	63.184	41.943	28.762	1.00	2.00	S
ATOM	212	C	LEU	36	62.119	38.179	26.803	1.00	2.00	S
ATOM	213	O	LEU	36	63.071	37.640	26.241	1.00	3.03	S
ATOM	214	N	VAL	37	61.038	38.589	26.151	1.00	3.65	S
ATOM	215	CA	VAL	37	60.960	38.559	24.707	1.00	3.46	7
ATOM	216	CB	VAL	37	59.866	37.575	24.268	1.00	2.30	S
ATOM	217	CG1	VAL	37	60.007	37.337	22.699	1.00	2.00	S
ATOM	218	CG2	VAL	37	59.957	36.271	24.942	1.00	2.00	S
ATOM	219	C	VAL	37	60.555	39.970	24.329	1.00	3.89	S
ATOM	220	O	VAL	37	59.738	40.553	25.042	1.00	5.63	S
ATOM	221	N	CYS	38	61.204	40.557	23.258	1.00	2.00	7
ATOM	222	CA	CYS	38	60.831	41.886	22.832	1.00	4.05	S
ATOM	223	C	CYS	38	60.762	41.816	21.324	1.00	5.14	S
ATOM	224	O	CYS	38	61.592	41.143	20.716	1.00	6.41	S
ATOM	225	CB	CYS	38	61.808	42.979	23.213	1.00	2.98	S
ATOM	226	SG	CYS	38	61.860	43.383	24.972	1.00	3.22	16

bref21c.pdb Thu Apr 25 12:27:47 1996 4

ATOM	227	N	PHE	39	59.811	42.540	30.742	1.00	4.35
ATOM	228	CA	PHE	39	59.621	42.507	29.286	1.00	5.38
ATOM	229	CB	PHE	39	58.865	41.225	28.900	1.00	4.80
ATOM	230	CG	PHE	39	57.461	41.198	29.411	1.00	7.09
ATOM	231	CD1	PHE	39	56.416	41.686	28.636	1.00	8.61
ATOM	232	CD2	PHE	39	57.190	40.807	30.709	1.00	7.97
ATOM	233	CE1	PHE	39	55.123	41.795	29.153	1.00	9.47
ATOM	234	CE2	PHE	39	55.896	40.917	31.228	1.00	9.36
ATOM	235	CZ	PHE	39	54.868	41.411	30.451	1.00	8.72
ATOM	236	C	PHE	39	58.826	43.713	28.794	1.00	3.79
ATOM	237	O	PHE	39	58.262	44.451	29.580	1.00	4.29
ATOM	238	N	TRP	40	58.837	43.926	27.490	1.00	3.45
ATOM	239	CA	TRP	40	58.084	44.996	26.846	1.00	4.71
ATOM	240	CB	TRP	40	58.826	46.352	26.872	1.00	4.45
ATOM	241	CG	TRP	40	60.014	46.517	25.928	1.00	7.44
ATOM	242	CD2	TRP	40	61.386	46.185	26.200	1.00	9.31
ATOM	243	CE2	TRP	40	62.143	46.555	25.062	1.00	6.04
ATOM	244	CE3	TRP	40	62.049	45.595	27.294	1.00	10.26
ATOM	245	CD1	TRP	40	60.003	47.056	24.661	1.00	8.12
ATOM	246	NE1	TRP	40	61.277	47.087	24.144	1.00	6.99
ATOM	247	CZ2	TRP	40	63.527	46.358	24.989	1.00	10.83
ATOM	248	CZ3	TRP	40	63.431	45.395	27.217	1.00	10.61
ATOM	249	CH2	TRP	40	64.152	45.780	26.068	1.00	11.48
ATOM	250	C	TRP	40	57.785	44.538	25.418	1.00	5.55
ATOM	251	O	TRP	40	58.530	43.761	24.824	1.00	4.51
ATOM	252	N	GLU	41	56.625	44.914	24.914	1.00	7.98
ATOM	253	CA	GLU	41	56.267	44.533	23.556	1.00	8.54
ATOM	254	CB	GLU	41	54.898	43.840	23.555	1.00	7.91
ATOM	255	CG	GLU	41	54.860	42.586	24.450	1.00	11.77
ATOM	256	CD	GLU	41	53.619	41.687	24.254	1.00	13.67
ATOM	257	OE1	GLU	41	53.418	40.748	25.055	1.00	15.11
ATOM	258	OE2	GLU	41	52.843	41.891	23.301	1.00	17.90
ATOM	259	C	GLU	41	56.335	45.715	22.558	1.00	9.08
ATOM	260	O	GLU	41	56.456	46.888	22.956	1.00	8.71
ATOM	261	N	GLU	42	56.403	45.389	21.271	1.00	8.40
ATOM	262	CA	GLU	42	56.426	46.399	20.211	1.00	8.84
ATOM	263	CB	GLU	42	57.729	47.207	20.227	1.00	6.56
ATOM	264	CG	GLU	42	58.974	46.393	20.511	1.00	5.92
ATOM	265	CD	GLU	42	60.242	47.114	20.115	1.00	7.01
ATOM	266	OE1	GLU	42	61.019	46.519	19.371	1.00	9.43
ATOM	267	OE2	GLU	42	60.470	48.271	20.519	1.00	6.18
ATOM	268	C	GLU	42	56.167	45.737	18.853	1.00	9.90
ATOM	269	O	GLU	42	55.880	44.532	18.795	1.00	9.59
ATOM	270	N	ALA	43	56.243	46.514	17.771	1.00	10.98
ATOM	271	CA	ALA	43	55.988	46.007	16.400	1.00	12.17
ATOM	272	CB	ALA	43	55.513	47.145	15.515	1.00	12.56
ATOM	273	C	ALA	43	57.164	45.291	15.731	1.00	10.71
ATOM	274	O	ALA	43	58.309	45.683	15.930	1.00	12.41
ATOM	275	N	ALA	44	56.878	44.282	14.903	1.00	9.23
ATOM	276	CA	ALA	44	57.928	43.514	14.208	1.00	8.12
ATOM	277	CB	ALA	44	57.326	42.507	13.263	1.00	4.97
ATOM	278	C	ALA	44	58.828	44.442	13.438	1.00	8.51
ATOM	279	O	ALA	44	58.407	45.534	13.047	1.00	9.87
ATOM	280	N	SER	45	60.086	44.068	13.275	1.00	9.06
ATOM	281	CA	SER	45	60.962	44.925	12.508	1.00	10.81
ATOM	282	CB	SER	45	61.618	46.002	13.354	1.00	11.34
ATOM	283	OG	SER	45	61.479	47.244	12.695	1.00	10.12
ATOM	284	C	SER	45	61.996	44.207	11.683	1.00	13.93
ATOM	285	O	SER	45	62.599	43.221	12.124	1.00	15.72
ATOM	286	N	ALA	46	62.112	44.671	10.435	1.00	14.88
ATOM	287	CA	ALA	46	63.041	44.134	9.469	1.00	14.41
ATOM	288	CB	ALA	46	62.810	44.781	8.127	1.00	17.01
ATOM	289	C	ALA	46	64.379	44.538	10.028	1.00	15.43
ATOM	290	O	ALA	46	64.657	45.746	10.203	1.00	16.67
ATOM	291	N	GLY	47	65.140	43.525	10.433	1.00	15.11
ATOM	292	CA	GLY	47	66.450	43.762	11.009	1.00	15.77
ATOM	293	C	GLY	47	66.558	44.415	12.400	1.00	15.18
ATOM	294	O	GLY	47	67.231	45.453	12.546	1.00	16.09
ATOM	295	N	VAL	48	65.872	43.843	13.399	1.00	13.87
ATOM	296	CA	VAL	48	65.950	44.202	14.799	1.00	11.89
ATOM	297	CB	VAL	48	64.825	45.230	15.231	1.00	8.24
ATOM	298	CG1	VAL	48	64.572	45.071	16.701	1.00	8.26
ATOM	299	CG2	VAL	48	65.216	46.656	14.964	1.00	8.13
ATOM	300	C	VAL	48	65.904	43.069	15.642	1.00	9.85
ATOM	301	O	VAL	48	65.062	42.183	15.443	1.00	9.93
ATOM	302	N	GLY	49	66.882	42.949	16.521	1.00	9.43
ATOM	303	CA	GLY	49	66.948	41.798	17.393	1.00	7.27
ATOM	304	C	GLY	49	67.199	42.211	18.829	1.00	5.14

ATOM	305	O	GLY	49	67.294	43.396	19.152	1.00	3.06	5
ATOM	306	N	PRO	50	67.274	41.234	19.732	1.00	4.49	7
ATOM	307	CD	PRO	50	67.104	39.790	19.536	1.00	2.00	6
ATOM	308	CA	PRO	50	67.519	41.540	21.125	1.00	2.99	6
ATOM	309	CB	PRO	50	67.545	40.158	21.762	1.00	3.97	6
ATOM	310	CG	PRO	50	67.935	39.264	20.632	1.00	2.00	6
ATOM	311	C	PRO	50	68.837	42.307	21.315	1.00	4.87	6
ATOM	312	O	PRO	50	68.962	43.122	22.217	1.00	7.36	8
ATOM	313	N	GLY	51	69.787	42.100	20.403	1.00	5.60	7
ATOM	314	CA	GLY	51	71.059	42.792	20.477	1.00	2.83	6
ATOM	315	C	GLY	51	70.991	44.263	20.103	1.00	3.36	6
ATOM	316	O	GLY	51	72.025	44.910	19.956	1.00	5.85	8
ATOM	317	N	ASN	52	69.792	44.815	19.968	1.00	2.00	7
ATOM	318	CA	ASN	52	69.670	46.211	19.604	1.00	2.00	6
ATOM	319	CB	ASN	52	68.527	46.401	18.633	1.00	3.33	6
ATOM	320	CG	ASN	52	68.768	47.534	17.666	1.00	7.97	6
ATOM	321	OD1	ASN	52	69.233	47.311	16.538	1.00	12.55	8
ATOM	322	ND2	ASN	52	68.442	48.753	18.079	1.00	10.05	7
ATOM	323	C	ASN	52	69.505	47.144	20.797	1.00	3.59	6
ATOM	324	O	ASN	52	69.524	48.359	20.638	1.00	2.00	8
ATOM	325	N	TYR	53	69.286	46.573	21.985	1.00	5.70	7
ATOM	326	CA	TYR	53	69.148	47.350	23.229	1.00	5.58	6
ATOM	327	CB	TYR	53	67.707	47.412	23.770	1.00	5.70	6
ATOM	328	CG	TYR	53	66.615	47.547	22.768	1.00	4.84	6
ATOM	329	CD1	TYR	53	66.067	46.414	22.188	1.00	6.02	6
ATOM	330	CE1	TYR	53	65.080	46.495	21.282	1.00	5.48	6
ATOM	331	CD2	TYR	53	66.123	48.789	22.405	1.00	5.30	6
ATOM	332	CE2	TYR	53	65.118	48.891	21.495	1.00	6.56	6
ATOM	333	CZ	TYR	53	64.598	47.729	20.929	1.00	8.17	6
ATOM	334	OH	TYR	53	63.590	47.767	19.987	1.00	12.54	8
ATOM	335	C	TYR	53	69.943	46.667	24.308	1.00	3.83	6
ATOM	336	O	TYR	53	70.176	45.465	24.245	1.00	4.09	8
ATOM	337	N	SER	54	70.257	47.428	25.346	1.00	3.81	7
ATOM	338	CA	SER	54	70.977	46.921	26.501	1.00	6.59	6
ATOM	339	CB	SER	54	72.296	47.682	26.710	1.00	8.72	6
ATOM	340	OG	SER	54	73.405	46.867	26.341	1.00	13.32	8
ATOM	341	C	SER	54	70.077	47.035	27.726	1.00	4.52	6
ATOM	342	O	SER	54	69.495	48.089	27.982	1.00	5.58	8
ATOM	343	N	PHE	55	69.931	45.926	28.443	1.00	3.52	7
ATOM	344	CA	PHE	55	69.095	45.878	29.641	1.00	3.38	6
ATOM	345	CB	PHE	55	68.141	44.676	29.574	1.00	6.11	6
ATOM	346	CG	PHE	55	67.052	44.700	30.596	1.00	6.96	6
ATOM	347	CD1	PHE	55	65.741	44.865	30.214	1.00	10.17	6
ATOM	348	CD2	PHE	55	67.330	44.547	31.929	1.00	8.73	6
ATOM	349	CE1	PHE	55	64.713	44.879	31.154	1.00	12.64	6
ATOM	350	CE2	PHE	55	66.317	44.561	32.874	1.00	8.02	6
ATOM	351	CZ	PHE	55	65.007	44.728	32.490	1.00	8.93	6
ATOM	352	C	PHE	55	69.942	45.779	30.891	1.00	2.90	6
ATOM	353	O	PHE	55	70.476	44.710	31.200	1.00	2.00	8
ATOM	354	N	SER	56	70.083	46.892	31.595	1.00	2.00	7
ATOM	355	CA	SER	56	70.854	46.862	32.818	1.00	5.40	6
ATOM	356	CB	SER	56	72.159	47.651	32.681	1.00	6.39	6
ATOM	357	OG	SER	56	71.950	48.939	32.162	1.00	9.05	8
ATOM	358	C	SER	56	70.089	47.214	34.108	1.00	8.43	6
ATOM	359	O	SER	56	69.080	47.943	34.098	1.00	7.21	8
ATOM	360	N	TYR	57	70.546	46.635	35.213	1.00	7.52	7
ATOM	361	CA	TYR	57	69.915	46.856	36.495	1.00	8.61	6
ATOM	362	CB	TYR	57	69.091	45.621	36.883	1.00	3.65	6
ATOM	363	CG	TYR	57	69.863	44.334	37.004	1.00	4.17	6
ATOM	364	CD1	TYR	57	70.254	43.825	38.254	1.00	2.00	6
ATOM	365	CE1	TYR	57	70.865	42.587	38.384	1.00	2.00	6
ATOM	366	CD2	TYR	57	70.115	43.560	35.894	1.00	4.11	6
ATOM	367	CE2	TYR	57	70.729	42.316	36.020	1.00	2.48	6
ATOM	368	CZ	TYR	57	71.096	41.834	37.260	1.00	2.00	6
ATOM	369	OH	TYR	57	71.672	40.591	37.334	1.00	2.00	8
ATOM	370	C	TYR	57	70.885	47.253	37.616	1.00	10.04	6
ATOM	371	O	TYR	57	72.092	47.181	37.466	1.00	11.97	8
ATOM	372	N	GLN	58	70.353	47.781	38.705	1.00	11.03	7
ATOM	373	CA	GLN	58	71.181	48.143	39.832	1.00	9.11	6
ATOM	374	CB	GLN	58	71.613	49.592	39.754	1.00	10.64	6
ATOM	375	CG	GLN	58	72.167	50.091	41.062	1.00	13.28	6
ATOM	376	CD	GLN	58	72.827	51.436	40.954	1.00	13.57	6
ATOM	377	OE1	GLN	58	72.165	52.472	40.844	1.00	15.62	8
ATOM	378	NE2	GLN	58	74.147	51.435	41.026	1.00	14.36	7
ATOM	379	C	GLN	58	70.630	47.886	41.123	1.00	8.05	6
ATOM	380	O	GLN	58	69.689	48.583	41.468	1.00	7.60	8
ATOM	381	N	LEU	59	70.737	46.798	41.769	1.00	8.41	7
ATOM	382	CA	LEU	59	70.183	46.435	43.038	1.00	8.43	6

bref21c.pdb Thu Apr 25 12:27:47 1996 6

ATOM	383	CB	LEU	59	70.534	44.993	43.313	1.00	4.10	6
ATOM	384	CG	LEU	59	69.811	44.304	44.446	1.00	2.46	6
ATOM	385	CD1	LEU	59	68.343	44.461	44.227	1.00	3.98	6
ATOM	386	CD2	LEU	59	70.246	42.909	44.462	1.00	6.03	6
ATOM	387	C	LEU	59	70.926	47.335	43.995	1.00	9.36	6
ATOM	388	O	LEU	59	72.125	47.210	44.085	1.00	9.93	8
ATOM	389	N	GLU	60	70.227	48.253	44.667	1.00	11.94	7
ATOM	390	CA	GLU	60	70.844	49.221	45.603	1.00	13.27	6
ATOM	391	CB	GLU	60	69.852	49.697	46.643	1.00	14.05	6
ATOM	392	CG	GLU	60	70.448	50.769	47.531	1.00	15.91	6
ATOM	393	CD	GLU	60	69.443	51.351	48.510	1.00	16.83	6
ATOM	394	OE1	GLU	60	69.263	50.755	49.607	1.00	16.52	8
ATOM	395	OE2	GLU	60	68.852	52.410	48.181	1.00	15.77	8
ATOM	396	C	GLU	60	72.159	48.859	46.315	1.00	14.73	6
ATOM	397	O	GLU	60	72.200	47.971	47.189	1.00	14.00	8
ATOM	398	N	ASP	61	73.193	49.638	45.973	1.00	16.22	7
ATOM	399	CA	ASP	61	74.569	49.501	46.452	1.00	17.32	6
ATOM	400	CB	ASP	61	74.624	49.151	47.930	1.00	22.61	6
ATOM	401	CG	ASP	61	74.287	50.345	48.814	1.00	26.60	6
ATOM	402	OD1	ASP	61	74.262	50.144	50.054	1.00	30.15	8
ATOM	403	OD2	ASP	61	74.036	51.470	48.271	1.00	27.62	8
ATOM	404	C	ASP	61	75.390	48.539	45.610	1.00	16.14	6
ATOM	405	O	ASP	61	76.582	48.742	45.423	1.00	16.58	8
ATOM	406	N	GLU	62	74.758	47.476	45.130	1.00	14.78	7
ATOM	407	CA	GLU	62	75.402	46.524	44.223	1.00	13.68	6
ATOM	408	CB	GLU	62	74.418	45.359	43.931	1.00	15.90	6
ATOM	409	CG	GLU	62	74.592	44.612	42.585	1.00	20.15	6
ATOM	410	CD	GLU	62	73.574	44.998	41.452	1.00	18.81	6
ATOM	411	OE1	GLU	62	73.324	46.202	41.202	1.00	19.09	8
ATOM	412	OE2	GLU	62	73.047	44.078	40.788	1.00	17.28	8
ATOM	413	C	GLU	62	75.709	47.363	42.947	1.00	10.99	6
ATOM	414	O	GLU	62	75.069	48.402	42.704	1.00	11.23	8
ATOM	415	N	PRO	63	76.744	46.984	42.173	1.00	9.01	7
ATOM	416	CD	PRO	63	77.785	45.973	42.435	1.00	9.66	6
ATOM	417	CA	PRO	63	77.069	47.740	40.959	1.00	8.47	6
ATOM	418	CB	PRO	63	78.517	47.322	40.691	1.00	5.33	6
ATOM	419	CG	PRO	63	78.504	45.895	41.103	1.00	7.09	6
ATOM	420	C	PRO	63	76.146	47.407	39.779	1.00	6.19	6
ATOM	421	O	PRO	63	75.473	46.366	39.775	1.00	4.91	8
ATOM	422	N	TRP	64	76.119	48.300	38.788	1.00	3.27	7
ATOM	423	CA	TRP	64	75.298	48.092	37.613	1.00	2.00	6
ATOM	424	CB	TRP	64	75.441	49.259	36.645	1.00	2.40	6
ATOM	425	CG	TRP	64	74.591	50.490	36.923	1.00	2.00	6
ATOM	426	CD2	TRP	64	73.181	50.651	36.678	1.00	2.00	6
ATOM	427	CE2	TRP	64	72.845	51.972	37.050	1.00	2.28	6
ATOM	428	CE3	TRP	64	72.174	49.811	36.186	1.00	2.18	6
ATOM	429	CD1	TRP	64	75.027	51.682	37.410	1.00	2.00	6
ATOM	430	NE1	TRP	64	73.995	52.573	37.487	1.00	2.00	7
ATOM	431	CZ2	TRP	64	71.537	52.476	36.950	1.00	2.00	6
ATOM	432	CZ3	TRP	64	70.878	50.314	36.087	1.00	2.49	6
ATOM	433	CH2	TRP	64	70.575	51.636	36.471	1.00	2.00	6
ATOM	434	C	TRP	64	75.700	46.815	36.903	1.00	2.00	6
ATOM	435	O	TRP	64	76.877	46.528	36.736	1.00	2.00	8
ATOM	436	N	LYS	65	74.704	46.036	36.524	1.00	2.00	7
ATOM	437	CA	LYS	65	74.909	44.793	35.803	1.00	2.00	6
ATOM	438	CB	LYS	65	74.603	43.597	36.668	1.00	2.61	6
ATOM	439	CG	LYS	65	75.611	43.306	37.673	1.00	3.35	6
ATOM	440	CD	LYS	65	75.207	42.082	38.401	1.00	4.33	6
ATOM	441	CE	LYS	65	76.204	41.795	39.488	1.00	10.13	6
ATOM	442	NZ	LYS	65	76.452	43.031	40.293	1.00	15.09	7
ATOM	443	C	LYS	65	74.017	44.725	34.584	1.00	2.00	6
ATOM	444	O	LYS	65	73.125	45.534	34.416	1.00	2.81	8
ATOM	445	N	LEU	66	74.201	43.692	33.780	1.00	2.51	7
ATOM	446	CA	LEU	66	73.421	43.532	32.558	1.00	3.38	6
ATOM	447	CB	LEU	66	74.342	43.585	31.340	1.00	2.07	6
ATOM	448	CG	LEU	66	75.135	44.851	31.138	1.00	2.42	6
ATOM	449	CD1	LEU	66	76.363	44.485	30.416	1.00	5.47	6
ATOM	450	CD2	LEU	66	74.327	45.880	30.283	1.00	2.99	6
ATOM	451	C	LEU	66	72.651	42.234	32.492	1.00	3.16	6
ATOM	452	O	LEU	66	73.125	41.195	32.943	1.00	2.56	8
ATOM	453	N	CYS	67	71.479	42.268	31.885	1.00	4.64	7
ATOM	454	CA	CYS	67	70.686	41.099	31.708	1.00	8.30	6
ATOM	455	C	CYS	67	70.569	40.352	30.191	1.00	9.34	6
ATOM	456	O	CYS	67	70.506	41.960	29.512	1.00	11.12	8
ATOM	457	CB	CYS	67	69.331	41.270	32.363	1.00	9.68	6
ATOM	458	SG	CYS	67	68.297	39.785	32.300	1.00	9.98	16
ATOM	459	N	ARG	68	70.672	39.729	29.649	1.00	10.38	7
ATOM	460	CA	ARG	68	70.567	39.534	28.187	1.00	11.77	6

ATOM	461	CB	ARG	68	71.380	38.359	27.627	1.00	15.15
ATOM	462	CG	ARG	68	71.366	38.376	26.053	1.00	20.38
ATOM	463	CD	ARG	68	71.858	37.102	25.359	1.00	21.17
ATOM	464	NE	ARG	68	71.010	35.943	25.653	1.00	25.20
ATOM	465	CZ	ARG	68	71.437	34.837	26.288	1.00	27.66
ATOM	466	NH1	ARG	68	72.710	34.732	26.705	1.00	28.62
ATOM	467	NH2	ARG	68	70.601	33.818	26.498	1.00	27.68
ATOM	468	C	ARG	68	69.143	39.327	27.751	1.00	9.76
ATOM	469	O	ARG	68	68.449	38.504	28.317	1.00	9.75
ATOM	470	N	LEU	69	68.762	40.027	26.684	1.00	8.16
ATOM	471	CA	LEU	69	67.428	39.983	26.131	1.00	5.24
ATOM	472	CB	LEU	69	67.137	41.247	25.328	1.00	4.64
ATOM	473	CG	LEU	69	67.431	42.587	25.980	1.00	5.82
ATOM	474	CD1	LEU	69	67.302	43.727	25.026	1.00	9.48
ATOM	475	CD2	LEU	69	66.498	42.773	27.111	1.00	9.06
ATOM	476	C	LEU	69	67.222	38.794	25.221	1.00	6.45
ATOM	477	O	LEU	69	68.175	38.217	24.655	1.00	6.60
ATOM	478	N	HIS	70	65.947	38.430	25.133	1.00	6.17
ATOM	479	CA	HIS	70	65.448	37.374	24.296	1.00	4.34
ATOM	480	CB	HIS	70	64.792	36.308	25.103	1.00	3.32
ATOM	481	CG	HIS	70	65.759	35.494	25.871	1.00	4.94
ATOM	482	CD2	HIS	70	66.779	34.706	25.460	1.00	7.46
ATOM	483	ND1	HIS	70	65.759	35.444	27.243	1.00	8.83
ATOM	484	CE1	HIS	70	66.738	34.653	27.650	1.00	9.22
ATOM	485	NE2	HIS	70	67.372	34.193	26.586	1.00	6.78
ATOM	486	C	HIS	70	64.407	38.097	23.546	1.00	6.62
ATOM	487	O	HIS	70	64.129	39.240	23.863	1.00	7.62
ATOM	488	N	GLN	71	63.871	37.453	22.520	1.00	10.06
ATOM	489	CA	GLN	71	62.826	36.028	21.676	1.00	12.44
ATOM	490	CB	GLN	71	63.449	38.691	20.442	1.00	12.64
ATOM	491	CG	GLN	71	62.523	39.628	19.675	1.00	12.33
ATOM	492	CD	GLN	71	63.193	40.157	18.423	1.00	11.98
ATOM	493	OE1	GLN	71	63.256	41.364	18.185	1.00	14.18
ATOM	494	NE2	GLN	71	63.741	39.254	17.638	1.00	13.04
ATOM	495	C	GLN	71	61.867	36.915	21.278	1.00	14.54
ATOM	496	O	GLN	71	62.293	35.846	20.828	1.00	13.15
ATOM	497	N	ALA	72	60.576	37.148	21.510	1.00	16.60
ATOM	498	CA	ALA	72	59.540	36.163	21.222	1.00	17.29
ATOM	499	CB	ALA	72	59.106	35.462	22.513	1.00	18.25
ATOM	500	C	ALA	72	58.339	36.816	20.552	1.00	17.09
ATOM	501	O	ALA	72	57.962	37.949	20.890	1.00	17.99
ATOM	502	N	PRO	73	57.770	36.140	19.535	1.00	15.70
ATOM	503	CD	PRO	73	58.266	34.944	18.833	1.00	15.56
ATOM	504	CA	PRO	73	56.618	36.681	18.835	1.00	14.26
ATOM	505	CB	PRO	73	56.539	35.789	17.608	1.00	14.62
ATOM	506	CG	PRO	73	57.057	34.500	18.096	1.00	14.52
ATOM	507	C	PRO	73	55.292	36.586	19.707	1.00	13.69
ATOM	508	O	PRO	73	55.295	35.678	20.522	1.00	16.10
ATOM	509	N	THR	74	54.568	37.632	19.628	1.00	12.65
ATOM	510	CA	THR	74	53.304	37.789	20.338	1.00	11.59
ATOM	511	CB	THR	74	52.987	39.276	20.518	1.00	8.94
ATOM	512	CG1	THR	74	54.100	39.935	21.092	1.00	12.22
ATOM	513	CG2	THR	74	51.790	39.484	21.423	1.00	13.10
ATOM	514	C	THR	74	52.216	37.289	19.382	1.00	13.56
ATOM	515	O	THR	74	52.234	37.637	18.198	1.00	16.99
ATOM	516	N	ALA	75	51.237	36.542	19.885	1.00	12.64
ATOM	517	CA	ALA	75	50.131	36.076	19.045	1.00	10.05
ATOM	518	CB	ALA	75	48.995	35.578	19.905	1.00	10.80
ATOM	519	C	ALA	75	49.612	37.152	18.102	1.00	8.70
ATOM	520	O	ALA	75	49.256	36.837	16.987	1.00	12.33
ATOM	521	N	ARG	76	49.583	38.410	18.545	1.00	9.12
ATOM	522	CA	ARG	76	49.107	39.552	17.744	1.00	10.37
ATOM	523	CB	ARG	76	48.870	40.786	18.606	1.00	10.98
ATOM	524	CG	ARG	76	47.709	40.722	19.529	1.00	16.38
ATOM	525	CD	ARG	76	47.936	41.676	20.736	1.00	21.72
ATOM	526	NE	ARG	76	47.298	41.163	21.957	1.00	23.03
ATOM	527	CZ	ARG	76	47.700	40.066	22.605	1.00	25.34
ATOM	528	NH1	ARG	76	48.745	39.355	22.162	1.00	25.68
ATOM	529	NH2	ARG	76	47.065	39.679	23.712	1.00	28.25
ATOM	530	C	ARG	76	50.026	40.042	16.641	1.00	12.35
ATOM	531	O	ARG	76	49.680	41.002	15.961	1.00	15.69
ATOM	532	N	GLY	77	51.223	39.489	16.508	1.00	12.77
ATOM	533	CA	GLY	77	52.121	39.982	15.473	1.00	11.89
ATOM	534	C	GLY	77	53.079	41.083	15.909	1.00	10.38
ATOM	535	O	GLY	77	53.633	41.814	15.102	1.00	10.58
ATOM	536	N	ALA	78	53.243	41.226	17.209	1.00	12.04
ATOM	537	CA	ALA	78	54.158	42.210	17.759	1.00	11.50
ATOM	538	CB	ALA	78	53.465	43.041	18.831	1.00	10.28

bref21c.pdb Thu Apr 25 12:27:47 1996 8

ATOM	539	C	ALA	78	55.263	41.329	18.357	1.00	11.11	6
ATOM	540	O	ALA	78	55.080	40.106	18.495	1.00	10.01	8
ATOM	541	N	VAL	79	56.418	41.923	18.640	1.00	9.69	7
ATOM	542	CA	VAL	79	57.546	41.178	19.192	1.00	7.82	6
ATOM	543	CB	VAL	79	58.844	41.391	18.354	1.00	6.05	6
ATOM	544	CG1	VAL	79	58.706	40.741	17.024	1.00	6.29	6
ATOM	545	CG2	VAL	79	59.135	42.848	18.171	1.00	5.80	6
ATOM	546	C	VAL	79	57.786	41.500	20.672	1.00	5.75	6
ATOM	547	O	VAL	79	57.633	42.637	21.125	1.00	4.75	8
ATOM	548	N	ARG	80	58.207	40.491	21.403	1.00	4.34	7
ATOM	549	CA	ARG	80	58.420	40.648	22.813	1.00	7.09	6
ATOM	550	CB	ARG	80	57.507	39.672	23.550	1.00	8.65	6
ATOM	551	CG	ARG	80	57.465	39.838	25.052	1.00	7.34	6
ATOM	552	CD	ARG	80	56.674	38.710	25.630	1.00	6.89	6
ATOM	553	NE	ARG	80	55.272	38.809	25.237	1.00	6.67	7
ATOM	554	CZ	ARG	80	54.415	37.809	25.313	1.00	4.11	6
ATOM	555	NH1	ARG	80	54.829	36.631	25.743	1.00	5.04	7
ATOM	556	NH2	ARG	80	53.142	38.017	25.063	1.00	2.00	7
ATOM	557	C	ARG	80	59.846	40.484	23.297	1.00	5.10	6
ATOM	558	O	ARG	80	60.466	39.434	23.114	1.00	3.87	8
ATOM	559	N	PHE	81	60.346	41.519	23.951	1.00	4.32	7
ATOM	560	CA	PHE	81	61.688	41.481	24.488	1.00	5.56	6
ATOM	561	CB	PHE	81	62.385	42.814	24.305	1.00	4.97	6
ATOM	562	CG	PHE	81	62.744	43.102	22.915	1.00	5.07	6
ATOM	563	CD1	PHE	81	61.861	43.781	22.091	1.00	6.98	6
ATOM	564	CD2	PHE	81	63.947	42.670	22.409	1.00	7.17	6
ATOM	565	CE1	PHE	81	62.164	44.030	20.763	1.00	7.58	6
ATOM	566	CE2	PHE	81	64.275	42.908	21.086	1.00	10.89	6
ATOM	567	CZ	PHE	81	63.374	43.594	20.251	1.00	10.08	6
ATOM	568	C	PHE	81	61.546	41.209	25.955	1.00	7.23	6
ATOM	569	O	PHE	81	60.725	41.848	26.604	1.00	8.68	8
ATOM	570	N	TRP	82	62.301	40.240	26.469	1.00	7.82	7
ATOM	571	CA	TRP	82	62.263	39.911	27.891	1.00	8.83	6
ATOM	572	CB	TRP	82	61.253	38.789	28.199	1.00	9.85	6
ATOM	573	CG	TRP	82	61.585	37.412	27.697	1.00	12.09	6
ATOM	574	CD2	TRP	82	62.234	36.372	28.428	1.00	11.52	6
ATOM	575	CE2	TRP	82	62.328	35.248	27.577	1.00	13.27	6
ATOM	576	CE3	TRP	82	62.744	36.277	29.722	1.00	15.01	6
ATOM	577	CD1	TRP	82	61.304	36.888	26.453	1.00	14.64	6
ATOM	578	NE1	TRP	82	61.750	35.581	26.378	1.00	12.57	7
ATOM	579	CZ2	TRP	82	62.919	34.048	27.987	1.00	17.05	6
ATOM	580	CZ3	TRP	82	63.333	35.071	30.137	1.00	16.75	6
ATOM	581	CH2	TRP	82	63.415	33.980	29.272	1.00	17.82	6
ATOM	582	C	TRP	82	63.656	39.561	28.371	1.00	8.05	6
ATOM	583	O	TRP	82	64.606	39.733	27.623	1.00	7.22	8
ATOM	584	N	CYS	83	63.769	39.156	29.635	1.00	7.16	7
ATOM	585	CA	CYS	83	65.024	38.749	30.282	1.00	6.82	6
ATOM	586	C	CYS	83	64.632	38.373	31.702	1.00	4.93	6
ATOM	587	O	CYS	83	63.737	38.969	32.271	1.00	5.96	8
ATOM	588	CB	CYS	83	66.026	39.909	30.319	1.00	7.79	6
ATOM	589	SG	CYS	83	66.435	40.538	31.992	1.00	15.35	16
ATOM	590	N	SER	84	65.241	37.353	32.258	1.00	3.11	7
ATOM	591	CA	SER	84	64.904	36.980	33.610	1.00	4.32	6
ATOM	592	CB	SER	84	64.396	35.555	33.658	1.00	5.70	6
ATOM	593	OG	SER	84	65.095	34.752	32.731	1.00	12.40	8
ATOM	594	C	SER	84	66.124	37.135	34.483	1.00	7.36	6
ATOM	595	O	SER	84	67.172	36.544	34.190	1.00	11.62	8
ATOM	596	N	LEU	85	66.002	37.940	35.546	1.00	7.67	7
ATOM	597	CA	LEU	85	67.115	38.209	36.457	1.00	4.88	6
ATOM	598	CB	LEU	85	66.677	39.160	37.546	1.00	3.56	6
ATOM	599	CG	LEU	85	66.732	40.624	37.197	1.00	5.43	6
ATOM	600	CD1	LEU	85	67.012	41.388	38.482	1.00	7.87	6
ATOM	601	CD2	LEU	85	67.840	40.844	35.232	1.00	6.46	6
ATOM	602	C	LEU	85	67.709	36.991	37.110	1.00	6.20	6
ATOM	603	O	LEU	85	67.002	36.021	37.352	1.00	9.21	8
ATOM	604	N	PRO	86	69.027	37.013	37.388	1.00	5.88	7
ATOM	605	CD	PRO	86	69.953	38.092	35.989	1.00	6.27	6
ATOM	606	CA	PRO	86	69.760	35.918	38.036	1.00	4.84	6
ATOM	607	CB	PRO	86	71.212	36.361	37.921	1.00	3.16	6
ATOM	608	CG	PRO	86	71.201	37.343	36.772	1.00	5.18	6
ATOM	609	C	PRO	86	69.332	35.832	39.515	1.00	3.99	6
ATOM	610	O	PRO	86	69.142	36.847	40.187	1.00	4.26	8
ATOM	611	N	THR	87	69.227	34.622	40.029	1.00	4.59	7
ATOM	612	CA	THR	87	68.792	34.399	41.394	1.00	6.71	6
ATOM	613	CB	THR	87	68.963	32.949	41.727	1.00	8.22	6
ATOM	614	OG1	THR	87	68.497	32.183	40.607	1.00	9.30	8
ATOM	615	CG2	THR	87	68.149	32.599	42.975	1.00	11.56	6
ATOM	616	C	THR	87	69.252	35.263	42.531	1.00	7.76	6

bref21c.pdb Thu Apr 25 12:27:47 1996 9

ATOM	617	O	THR	87	68.606	35.730	43.384	1.00	9.13	
ATOM	618	N	ALA	88	70.661	35.474	42.541	1.00	8.99	
ATOM	619	CA	ALA	88	71.313	36.286	43.568	1.00	8.39	
ATOM	620	CB	ALA	88	72.812	36.176	43.419	1.00	9.06	
ATOM	621	C	ALA	88	70.922	37.752	43.497	1.00	8.97	
ATOM	622	O	ALA	88	71.441	38.573	44.247	1.00	10.83	
ATOM	623	N	ASP	89	70.030	38.090	42.578	1.00	8.36	
ATOM	624	CA	ASP	89	69.633	39.470	42.397	1.00	8.96	
ATOM	625	CB	ASP	89	70.047	39.911	40.992	1.00	7.68	
ATOM	626	CG	ASP	89	71.563	39.915	40.788	1.00	6.73	
ATOM	627	OD1	ASP	89	72.319	40.224	41.720	1.00	8.92	
ATOM	628	OD2	ASP	89	72.012	39.646	39.667	1.00	6.25	
ATOM	629	C	ASP	89	68.141	39.746	42.654	1.00	9.65	
ATOM	630	O	ASP	89	67.668	40.880	42.522	1.00	9.22	
ATOM	631	N	THR	90	67.420	38.724	43.094	1.00	7.69	
ATOM	632	CA	THR	90	66.010	38.866	43.359	1.00	5.03	
ATOM	633	CB	THR	90	65.298	37.603	42.898	1.00	3.78	
ATOM	634	OG1	THR	90	65.905	36.466	43.495	1.00	2.00	
ATOM	635	CG2	THR	90	65.464	37.445	41.430	1.00	3.18	
ATOM	636	C	THR	90	65.667	39.219	44.823	1.00	8.87	
ATOM	637	O	THR	90	64.634	38.790	45.335	1.00	11.62	
ATOM	638	N	SER	91	66.492	40.043	45.479	1.00	7.49	
ATOM	639	CA	SER	91	66.264	40.434	46.877	1.00	7.31	
ATOM	640	CB	SER	91	67.470	41.178	47.448	1.00	9.23	
ATOM	641	OG	SER	91	68.619	40.343	47.478	1.00	9.38	
ATOM	642	C	SER	91	65.008	41.265	47.033	1.00	8.55	
ATOM	643	O	SER	91	64.779	42.197	46.263	1.00	9.93	
ATOM	644	N	SER	92	64.287	41.029	48.125	1.00	8.52	
ATOM	645	CA	SER	92	63.000	41.671	48.338	1.00	6.55	
ATOM	646	CB	SER	92	62.022	40.702	49.003	1.00	7.73	
ATOM	647	OG	SER	92	61.127	40.120	48.085	1.00	9.02	
ATOM	648	C	SER	92	62.732	42.992	48.963	1.00	6.08	
ATOM	649	O	SER	92	61.652	43.499	48.744	1.00	10.02	
ATOM	650	N	PHE	93	63.600	43.581	49.764	1.00	5.40	
ATOM	651	CA	PHE	93	63.132	44.847	50.366	1.00	3.55	
ATOM	652	CB	PHE	93	62.881	44.663	51.879	1.00	2.38	
ATOM	653	CG	PHE	93	61.836	43.585	52.207	1.00	2.00	
ATOM	654	CD1	PHE	93	62.214	42.264	52.444	1.00	2.00	
ATOM	655	CD2	PHE	93	60.475	43.884	52.232	1.00	2.00	
ATOM	656	CE1	PHE	93	61.260	41.265	52.689	1.00	2.00	
ATOM	657	CE2	PHE	93	59.520	42.881	52.478	1.00	2.00	
ATOM	658	CZ	PHE	93	59.922	41.573	52.704	1.00	2.00	
ATOM	659	C	PHE	93	63.923	46.107	50.035	1.00	5.65	
ATOM	660	O	PHE	93	63.753	47.156	50.657	1.00	5.77	
ATOM	661	N	VAL	94	64.671	46.008	48.938	1.00	5.76	
ATOM	662	CA	VAL	94	65.542	47.054	48.410	1.00	4.07	
ATOM	663	CB	VAL	94	66.969	46.501	48.238	1.00	3.20	
ATOM	664	CG1	VAL	94	67.600	46.310	49.571	1.00	6.25	
ATOM	665	CG2	VAL	94	66.935	45.177	47.522	1.00	2.00	
ATOM	666	C	VAL	94	65.042	47.525	47.040	1.00	6.50	
ATOM	667	O	VAL	94	64.317	46.793	46.368	1.00	6.26	
ATOM	668	N	PRO	95	65.364	48.780	46.648	1.00	4.63	
ATOM	669	CD	PRO	95	65.947	49.823	47.507	1.00	5.07	
ATOM	670	CA	PRO	95	64.960	49.357	45.365	1.00	2.90	
ATOM	671	CB	PRO	95	65.316	50.826	45.530	1.00	2.93	
ATOM	672	CG	PRO	95	65.261	51.036	47.004	1.00	4.40	
ATOM	673	C	PRO	95	65.783	48.756	44.248	1.00	5.07	
ATOM	674	O	PRO	95	66.985	48.592	44.399	1.00	7.49	
ATOM	675	N	LEU	96	65.128	48.419	43.141	1.00	6.65	
ATOM	676	CA	LEU	96	65.776	47.852	41.957	1.00	5.19	
ATOM	677	CB	LEU	96	65.088	46.531	41.543	1.00	3.04	
ATOM	678	CG	LEU	96	65.571	45.607	40.411	1.00	2.00	
ATOM	679	CD1	LEU	96	66.945	45.060	40.642	1.00	2.00	
ATOM	680	CD2	LEU	96	64.648	44.446	40.315	1.00	2.00	
ATOM	681	C	LEU	96	65.713	48.886	43.816	1.00	5.21	
ATOM	682	O	LEU	96	64.639	49.309	40.367	1.00	5.02	
ATOM	683	N	GLU	97	66.881	49.355	40.416	1.00	8.18	
ATOM	684	CA	GLU	97	67.000	50.324	39.336	1.00	8.49	
ATOM	685	CB	GLU	97	68.315	51.069	39.476	1.00	10.17	
ATOM	686	CG	GLU	97	68.162	52.499	39.849	1.00	10.56	
ATOM	687	CD	GLU	97	67.806	53.335	38.676	1.00	12.04	
ATOM	688	OE1	GLU	97	68.087	54.545	38.734	1.00	14.20	
ATOM	689	OE2	GLU	97	67.252	52.787	37.691	1.00	17.92	
ATOM	690	C	GLU	97	66.959	49.610	37.387	1.00	8.71	
ATOM	691	O	GLU	97	67.735	48.689	37.741	1.00	9.01	
ATOM	692	N	LEU	98	66.083	50.053	37.101	1.00	8.76	
ATOM	693	CA	LEU	98	65.954	49.400	35.821	1.00	8.77	
ATOM	694	CB	LEU	98	64.592	48.695	35.754	1.00	8.21	

bref21c.pdb Thu Apr 25 12:27:47 1996 10

ATOM	695	CG	LEU	98	64.366	47.487	35.686	1.00	9.97	
ATOM	696	CD1	LEU	98	62.912	47.080	36.721	1.00	9.15	
ATOM	697	CD2	LEU	98	65.203	46.309	35.266	1.00	9.89	
ATOM	698	C	LEU	98	66.141	50.388	34.676	1.00	9.74	
ATOM	699	O	LEU	98	65.751	51.556	34.781	1.00	11.17	
ATOM	700	N	ARG	99	66.814	49.945	33.621	1.00	7.82	
ATOM	701	CA	ARG	99	67.050	50.799	32.467	1.00	8.42	
ATOM	702	CB	ARG	99	68.265	51.701	32.680	1.00	9.99	
ATOM	703	CG	ARG	99	68.319	52.571	33.915	1.00	13.57	
ATOM	704	CD	ARG	99	69.548	53.483	33.822	1.00	15.65	
ATOM	705	NE	ARG	99	70.798	52.717	33.766	1.00	21.42	
ATOM	706	CZ	ARG	99	71.623	52.634	32.709	1.00	23.75	
ATOM	707	NH1	ARG	99	71.364	53.271	31.557	1.00	25.09	
ATOM	708	NH2	ARG	99	72.747	51.921	32.818	1.00	24.11	
ATOM	709	C	ARG	99	67.294	50.002	31.174	1.00	7.64	
ATOM	710	O	ARG	99	68.179	49.159	31.118	1.00	8.53	
ATOM	711	N	VAL	100	66.528	50.307	30.136	1.00	5.56	
ATOM	712	CA	VAL	100	66.670	49.664	28.852	1.00	5.54	
ATOM	713	CB	VAL	100	65.321	49.097	28.397	1.00	8.61	
ATOM	714	CG1	VAL	100	65.446	48.467	27.008	1.00	7.63	
ATOM	715	CG2	VAL	100	64.821	48.100	29.419	1.00	7.70	
ATOM	716	C	VAL	100	67.146	50.745	27.877	1.00	6.61	
ATOM	717	O	VAL	100	66.556	51.831	27.819	1.00	3.63	
ATOM	718	N	THR	101	68.236	50.490	27.156	1.00	7.98	
ATOM	719	CA	THR	101	68.768	51.483	26.193	1.00	10.18	
ATOM	720	CB	THR	101	70.000	52.277	26.748	1.00	8.43	
ATOM	721	OG1	THR	101	70.526	51.629	27.908	1.00	13.91	
ATOM	722	CG2	THR	101	69.603	53.662	27.148	1.00	11.20	
ATOM	723	C	THR	101	69.115	50.926	24.792	1.00	11.66	
ATOM	724	O	THR	101	69.483	49.758	24.645	1.00	11.61	
ATOM	725	N	ALA	102	68.915	51.752	23.767	1.00	12.50	
ATOM	726	CA	ALA	102	69.216	51.369	22.386	1.00	14.07	
ATOM	727	CB	ALA	102	68.735	52.465	21.399	1.00	14.73	
ATOM	728	C	ALA	102	70.721	51.154	22.249	1.00	13.24	
ATOM	729	O	ALA	102	71.511	51.752	23.012	1.00	12.22	
ATOM	730	N	ALA	103	71.111	50.332	21.270	1.00	12.73	
ATOM	731	CA	ALA	103	72.520	50.004	21.021	1.00	13.74	
ATOM	732	CB	ALA	103	72.631	48.712	20.183	1.00	15.06	
ATOM	733	C	ALA	103	73.250	51.173	20.338	1.00	14.07	
ATOM	734	O	ALA	103	73.958	51.013	19.345	1.00	16.53	
ATOM	735	N	SER	104	73.105	52.341	20.931	1.00	12.51	
ATOM	736	CA	SER	104	73.673	53.569	20.440	1.00	10.25	
ATOM	737	CB	SER	104	72.834	54.066	19.266	1.00	9.41	
ATOM	738	OG	SER	104	71.434	54.033	19.565	1.00	8.47	
ATOM	739	C	SER	104	73.507	54.528	21.600	1.00	11.58	
ATOM	740	O	SER	104	73.557	55.746	21.412	1.00	11.80	
ATOM	741	N	GLY	105	73.187	53.964	22.770	1.00	11.41	
ATOM	742	CA	GLY	105	73.002	54.747	23.976	1.00	12.64	
ATOM	743	C	GLY	105	71.737	55.568	23.980	1.00	13.51	
ATOM	744	O	GLY	105	71.507	56.335	24.921	1.00	15.64	
ATOM	745	N	ALA	106	70.929	55.433	22.930	1.00	12.54	
ATOM	746	CA	ALA	106	69.668	56.166	22.837	1.00	11.65	
ATOM	747	CB	ALA	106	69.068	56.040	21.444	1.00	13.77	
ATOM	748	C	ALA	106	68.752	55.553	23.884	1.00	11.28	
ATOM	749	O	ALA	106	68.501	54.338	23.899	1.00	10.70	
ATOM	750	N	PRO	107	68.239	56.392	24.779	1.00	8.60	
ATOM	751	CD	PRO	107	68.390	57.855	24.666	1.00	9.28	
ATOM	752	CA	PRO	107	67.354	56.019	25.882	1.00	7.77	
ATOM	753	CB	PRO	107	67.282	57.314	26.683	1.00	8.42	
ATOM	754	CG	PRO	107	67.302	58.359	25.605	1.00	9.15	
ATOM	755	C	PRO	107	65.964	55.453	25.552	1.00	7.66	
ATOM	756	O	PRO	107	65.224	56.048	24.761	1.00	8.78	
ATOM	757	N	ARG	108	65.595	54.352	26.196	1.00	7.20	
ATOM	758	CA	ARG	108	64.290	53.751	25.990	1.00	4.63	
ATOM	759	CB	ARG	108	64.439	52.415	25.258	1.00	7.42	
ATOM	760	CG	ARG	108	63.168	51.902	24.695	1.00	10.88	
ATOM	761	CD	ARG	108	62.782	52.688	23.460	1.00	14.12	
ATOM	762	NE	ARG	108	61.461	52.313	22.964	1.00	16.25	
ATOM	763	CZ	ARG	108	61.086	51.084	22.650	1.00	15.01	
ATOM	764	NH1	ARG	108	61.917	50.067	22.764	1.00	18.31	
ATOM	765	NH2	ARG	108	59.858	50.867	22.236	1.00	19.47	
ATOM	766	C	ARG	108	63.455	53.624	27.253	1.00	5.36	
ATOM	767	O	ARG	108	62.420	54.259	27.404	1.00	4.86	
ATOM	768	N	TYR	109	63.863	52.827	28.263	1.00	6.12	
ATOM	769	CA	TYR	109	63.102	52.711	29.509	1.00	6.72	
ATOM	770	CB	TYR	109	62.419	51.350	29.631	1.00	7.62	
ATOM	771	CG	TYR	109	61.455	51.024	28.544	1.00	8.20	
ATOM	772	CD1	TYR	109	61.775	50.089	27.565	1.00	11.38	

ATOM	773	CE1	TYR	109	60.897	49.788	26.557	1.00	12.39	6
ATOM	774	CD2	TYR	109	60.230	51.642	28.480	1.00	10.61	6
ATOM	775	CE2	TYR	109	59.337	51.347	27.476	1.00	12.42	6
ATOM	776	CZ	TYR	109	59.670	50.421	26.511	1.00	12.48	6
ATOM	777	OH	TYR	109	58.777	50.152	25.481	1.00	14.44	8
ATOM	778	C	TYR	109	63.911	52.909	30.774	1.00	8.52	6
ATOM	779	O	TYR	109	65.124	52.737	30.794	1.00	9.59	8
ATOM	780	N	HIS	110	63.198	53.259	31.835	1.00	10.99	7
ATOM	781	CA	HIS	110	63.760	53.467	33.174	1.00	14.45	6
ATOM	782	CB	HIS	110	64.468	54.830	33.296	1.00	16.04	6
ATOM	783	CG	HIS	110	65.167	55.029	34.613	1.00	21.12	6
ATOM	784	CD2	HIS	110	66.383	54.616	35.048	1.00	21.71	6
ATOM	785	ND1	HIS	110	64.623	55.764	35.652	1.00	24.07	7
ATOM	786	CE1	HIS	110	65.476	55.803	36.662	1.00	23.40	6
ATOM	787	NE2	HIS	110	66.553	55.114	36.321	1.00	22.60	7
ATOM	788	C	HIS	110	62.628	53.380	34.214	1.00	12.21	6
ATOM	789	O	HIS	110	61.740	54.224	34.240	1.00	13.06	8
ATOM	790	N	ARG	111	62.693	52.361	35.062	1.00	11.08	7
ATOM	791	CA	ARG	111	61.716	52.116	36.112	1.00	10.30	6
ATOM	792	CB	ARG	111	60.878	50.881	35.742	1.00	9.90	6
ATOM	793	CG	ARG	111	59.700	50.590	36.641	1.00	8.05	6
ATOM	794	CD	ARG	111	58.370	50.465	35.862	1.00	8.40	6
ATOM	795	NE	ARG	111	57.828	49.099	35.783	1.00	8.93	7
ATOM	796	CZ	ARG	111	57.096	48.521	36.730	1.00	8.80	6
ATOM	797	NH1	ARG	111	56.822	49.182	37.840	1.00	10.13	7
ATOM	798	NH2	ARG	111	56.585	47.308	36.550	1.00	10.84	7
ATOM	799	C	ARG	111	62.546	51.850	37.369	1.00	11.27	6
ATOM	800	O	ARG	111	63.776	51.808	37.306	1.00	13.11	8
ATOM	801	N	VAL	112	61.877	51.758	38.510	1.00	11.56	7
ATOM	802	CA	VAL	112	62.493	51.471	39.822	1.00	11.15	6
ATOM	803	CB	VAL	112	62.882	52.803	40.601	1.00	12.50	6
ATOM	804	CG1	VAL	112	63.003	52.545	42.094	1.00	13.08	6
ATOM	805	CG2	VAL	112	64.235	53.354	40.093	1.00	12.31	6
ATOM	806	C	VAL	112	61.398	50.668	40.542	1.00	7.77	6
ATOM	807	O	VAL	112	60.268	51.105	40.581	1.00	8.50	8
ATOM	808	N	ILE	113	61.709	49.480	41.049	1.00	5.20	7
ATOM	809	CA	ILE	113	60.692	48.638	41.686	1.00	6.80	6
ATOM	810	CB	ILE	113	60.223	47.527	40.688	1.00	5.60	6
ATOM	811	CG2	ILE	113	59.680	48.130	39.426	1.00	6.45	6
ATOM	812	CG1	ILE	113	61.396	46.623	40.315	1.00	7.39	6
ATOM	813	CD1	ILE	113	61.012	45.471	39.468	1.00	9.87	6
ATOM	814	C	ILE	113	61.105	47.931	43.001	1.00	7.16	6
ATOM	815	O	ILE	113	62.141	48.234	43.572	1.00	9.02	8
ATOM	816	N	HIS	114	60.267	47.000	43.463	1.00	2.78	7
ATOM	817	CA	HIS	114	60.503	46.187	44.645	1.00	2.00	6
ATOM	818	CB	HIS	114	59.793	46.758	45.860	1.00	2.00	6
ATOM	819	CG	HIS	114	60.554	47.827	46.585	1.00	2.00	6
ATOM	820	CD2	HIS	114	61.337	47.787	47.652	1.00	4.32	6
ATOM	821	ND1	HIS	114	60.589	49.130	46.106	1.00	4.03	7
ATOM	822	CE1	HIS	114	61.368	49.850	46.891	1.00	2.34	6
ATOM	823	NE2	HIS	114	61.835	49.057	47.838	1.00	8.31	7
ATOM	824	C	HIS	114	59.907	44.830	44.330	1.00	2.00	6
ATOM	825	O	HIS	114	58.705	44.688	44.221	1.00	2.00	8
ATOM	826	N	ILE	115	60.741	43.820	44.201	1.00	2.00	7
ATOM	827	CA	ILE	115	60.261	42.495	43.871	1.00	2.00	6
ATOM	828	CB	ILE	115	61.439	41.480	43.883	1.00	3.84	6
ATOM	829	CG2	ILE	115	60.953	40.049	43.984	1.00	4.23	6
ATOM	830	CG1	ILE	115	62.333	41.672	42.650	1.00	2.00	6
ATOM	831	CD1	ILE	115	63.731	42.190	42.966	1.00	2.23	6
ATOM	832	C	ILE	115	59.107	42.012	44.751	1.00	3.56	6
ATOM	833	O	ILE	115	58.294	41.217	44.302	1.00	6.91	8
ATOM	834	N	ASN	116	59.013	42.492	45.989	1.00	4.63	7
ATOM	835	CA	ASN	116	57.936	42.066	46.895	1.00	5.21	6
ATOM	836	CB	ASN	116	58.317	42.342	48.370	1.00	5.23	6
ATOM	837	CG	ASN	116	58.582	43.823	48.655	1.00	5.84	6
ATOM	838	OD1	ASN	116	59.470	44.421	48.070	1.00	8.06	8
ATOM	839	ND2	ASN	116	57.806	44.414	49.551	1.00	8.46	7
ATOM	840	C	ASN	116	56.589	42.722	46.547	1.00	5.92	6
ATOM	841	O	ASN	116	55.512	42.223	46.879	1.00	4.52	8
ATOM	842	N	GLU	117	56.664	43.858	45.841	1.00	8.36	7
ATOM	843	CA	GLU	117	55.480	44.614	45.436	1.00	7.65	6
ATOM	844	CB	GLU	117	55.732	46.119	45.534	1.00	6.11	6
ATOM	845	CG	GLU	117	55.958	46.606	46.937	1.00	12.42	6
ATOM	846	CD	GLU	117	56.160	48.099	47.002	1.00	15.01	6
ATOM	847	OE1	GLU	117	56.648	48.691	48.056	1.00	18.35	8
ATOM	848	OE2	GLU	117	55.816	48.757	46.002	1.00	15.71	8
ATOM	849	C	GLU	117	55.116	44.321	44.025	1.00	6.25	6
ATOM	850	O	GLU	117	54.440	45.123	43.428	1.00	9.90	8

bref21c.pdb Thu Apr 25 12:27:47 1996 12

ATOM	851	N	VAL	118	55.477	43.151	43.523	1.00	3.55	
ATOM	852	CA	VAL	118	55.226	42.839	42.137	1.00	2.91	
ATOM	853	CB	VAL	118	56.373	43.488	41.261	1.00	2.00	
ATOM	854	CG1	VAL	118	57.484	42.519	40.942	1.00	2.85	
ATOM	855	CG2	VAL	118	55.828	44.165	40.062	1.00	2.00	
ATOM	856	C	VAL	118	55.060	41.334	41.948	1.00	2.18	
ATOM	857	O	VAL	118	55.453	40.755	40.936	1.00	3.50	
ATOM	858	N	VAL	119	54.404	40.716	42.919	1.00	2.79	
ATOM	859	CA	VAL	119	54.155	39.276	42.896	1.00	3.05	
ATOM	860	CB	VAL	119	53.776	38.736	44.305	1.00	2.45	
ATOM	861	CG1	VAL	119	53.749	37.267	44.292	1.00	2.00	
ATOM	862	CG2	VAL	119	54.735	39.231	45.352	1.00	2.00	
ATOM	863	C	VAL	119	52.998	38.960	41.945	1.00	2.00	
ATOM	864	O	VAL	119	52.007	39.674	41.932	1.00	2.00	
ATOM	865	N	LEU	120	53.171	37.919	41.132	1.00	3.02	
ATOM	866	CA	LEU	120	52.175	37.411	40.174	1.00	2.95	
ATOM	867	CB	LEU	120	52.446	37.894	38.745	1.00	5.65	
ATOM	868	CG	LEU	120	51.496	37.332	37.674	1.00	11.07	
ATOM	869	CD1	LEU	120	50.125	37.938	37.790	1.00	9.95	
ATOM	870	CD2	LEU	120	52.053	37.605	36.306	1.00	11.67	
ATOM	871	C	LEU	120	52.289	35.887	40.262	1.00	2.40	
ATOM	872	O	LEU	120	52.985	35.241	39.487	1.00	2.00	
ATOM	873	N	LEU	121	51.600	35.340	41.250	1.00	2.39	
ATOM	874	CA	LEU	121	51.629	33.924	41.552	1.00	2.77	
ATOM	875	CB	LEU	121	51.063	33.689	42.964	1.00	4.57	
ATOM	876	CG	LEU	121	52.050	33.227	44.062	1.00	10.24	
ATOM	877	CD1	LEU	121	52.939	32.076	43.550	1.00	14.87	
ATOM	878	CD2	LEU	121	52.944	34.328	44.501	1.00	9.45	
ATOM	879	C	LEU	121	50.974	32.995	40.554	1.00	5.41	
ATOM	880	O	LEU	121	50.256	33.420	39.654	1.00	7.50	
ATOM	881	N	ASP	122	51.279	31.709	40.672	1.00	8.57	
ATOM	882	CA	ASP	122	50.687	30.726	39.782	1.00	6.90	
ATOM	883	CB	ASP	122	51.493	29.421	39.773	1.00	7.76	
ATOM	884	CG	ASP	122	52.701	29.437	38.795	1.00	9.54	
ATOM	885	OD1	ASP	122	52.927	30.429	38.066	1.00	9.98	
ATOM	886	OD2	ASP	122	53.411	28.405	38.748	1.00	10.20	
ATOM	887	C	ASP	122	49.292	30.494	40.343	1.00	7.04	
ATOM	888	O	ASP	122	48.957	30.954	41.453	1.00	5.44	
ATOM	889	N	ALA	123	48.464	29.813	39.568	1.00	6.22	
ATOM	890	CA	ALA	123	47.107	29.562	40.010	1.00	4.76	
ATOM	891	CB	ALA	123	46.187	29.374	38.839	1.00	2.00	
ATOM	892	C	ALA	123	46.981	28.398	40.954	1.00	3.93	
ATOM	893	O	ALA	123	47.826	27.484	40.971	1.00	5.37	
ATOM	894	N	PRO	124	45.979	28.490	41.846	1.00	2.51	
ATOM	895	CD	PRO	124	45.216	29.736	42.096	1.00	2.90	
ATOM	896	CA	PRO	124	45.652	27.478	42.845	1.00	2.91	
ATOM	897	CB	PRO	124	44.362	28.022	43.436	1.00	2.00	
ATOM	898	CG	PRO	124	44.602	29.485	43.432	1.00	2.00	
ATOM	899	C	PRO	124	45.451	26.111	42.172	1.00	2.00	
ATOM	900	O	PRO	124	45.289	26.022	40.966	1.00	2.00	
ATOM	901	N	VAL	125	45.524	25.042	42.944	1.00	2.31	
ATOM	902	CA	VAL	125	45.345	23.715	42.381	1.00	4.06	
ATOM	903	CB	VAL	125	46.724	23.006	42.025	1.00	2.00	
ATOM	904	CG1	VAL	125	47.474	23.806	40.974	1.00	2.00	
ATOM	905	CG2	VAL	125	47.584	22.776	43.256	1.00	2.00	
ATOM	906	C	VAL	125	44.436	22.838	43.267	1.00	5.51	
ATOM	907	O	VAL	125	44.002	23.281	44.316	1.00	6.39	
ATOM	908	N	GLY	126	44.068	21.661	42.768	1.00	5.29	
ATOM	909	CA	GLY	126	43.230	20.735	43.494	1.00	4.13	
ATOM	910	C	GLY	126	41.939	21.283	44.035	1.00	5.54	
ATOM	911	O	GLY	126	41.588	20.981	45.170	1.00	8.57	
ATOM	912	N	LEU	127	41.246	22.112	43.268	1.00	5.83	
ATOM	913	CA	LEU	127	39.971	22.667	43.718	1.00	7.87	
ATOM	914	CB	LEU	127	39.594	23.949	42.935	1.00	9.72	
ATOM	915	CG	LEU	127	38.175	24.573	43.071	1.00	11.14	
ATOM	916	CD1	LEU	127	37.954	25.322	44.424	1.00	9.43	
ATOM	917	CD2	LEU	127	37.942	25.516	41.892	1.00	10.21	
ATOM	918	C	LEU	127	38.846	21.623	43.612	1.00	6.88	
ATOM	919	O	LEU	127	38.585	21.083	42.538	1.00	6.56	
ATOM	920	N	VAL	128	38.177	21.369	44.737	1.00	7.08	
ATOM	921	CA	VAL	128	37.087	20.406	44.815	1.00	6.92	
ATOM	922	CB	VAL	128	37.485	19.147	45.616	1.00	7.17	
ATOM	923	CG1	VAL	128	37.999	18.089	44.701	1.00	7.25	
ATOM	924	CG2	VAL	128	38.521	19.477	46.659	1.00	9.71	
ATOM	925	C	VAL	128	35.862	21.001	45.470	1.00	5.47	
ATOM	926	O	VAL	128	35.973	21.795	46.374	1.00	6.97	
ATOM	927	N	ALA	129	34.691	20.574	45.031	1.00	7.13	
ATOM	928	CA	ALA	129	33.430	21.061	45.579	1.00	6.61	

ATOM	929	CB	ALA	129	32.585	21.680	44.477	1.00	4.36	6
ATOM	930	C	ALA	129	32.693	19.876	46.202	1.00	9.11	6
ATOM	931	O	ALA	129	32.730	18.760	45.655	1.00	9.32	8
ATOM	932	N	ARG	130	32.018	20.106	47.329	1.00	9.76	7
ATOM	933	CA	ARG	130	31.288	19.020	47.990	1.00	10.55	6
ATOM	934	CB	ARG	130	32.220	18.310	48.967	1.00	11.88	6
ATOM	935	CG	ARG	130	31.765	16.979	49.486	1.00	11.87	6
ATOM	936	CD	ARG	130	32.108	16.871	50.963	1.00	15.67	6
ATOM	937	NE	ARG	130	33.351	17.567	51.252	1.00	15.76	7
ATOM	938	CZ	ARG	130	33.669	18.135	52.414	1.00	20.46	6
ATOM	939	NH1	ARG	130	32.818	18.092	53.449	1.00	18.08	7
ATOM	940	NH2	ARG	130	34.840	18.791	52.514	1.00	21.04	7
ATOM	941	C	ARG	130	30.028	19.479	48.721	1.00	10.90	6
ATOM	942	O	ARG	130	29.932	20.593	49.250	1.00	10.77	8
ATOM	943	N	LEU	131	29.065	18.582	48.792	1.00	12.00	7
ATOM	944	CA	LEU	131	27.813	18.909	49.460	1.00	13.66	6
ATOM	945	CB	LEU	131	26.640	18.313	48.688	1.00	12.73	6
ATOM	946	CG	LEU	131	25.301	18.517	49.353	1.00	11.96	6
ATOM	947	CD1	LEU	131	25.035	20.002	49.487	1.00	10.47	6
ATOM	948	CD2	LEU	131	24.252	17.783	48.531	1.00	11.69	6
ATOM	949	C	LEU	131	27.799	18.409	50.892	1.00	13.46	6
ATOM	950	O	LEU	131	27.702	17.204	51.128	1.00	12.81	8
ATOM	951	N	ALA	132	27.968	19.328	51.834	1.00	14.88	7
ATOM	952	CA	ALA	132	27.964	18.982	53.249	1.00	16.22	6
ATOM	953	CB	ALA	132	28.272	20.228	54.122	1.00	14.97	6
ATOM	954	C	ALA	132	26.638	18.324	53.656	1.00	16.57	6
ATOM	955	O	ALA	132	25.719	19.000	54.109	1.00	16.97	8
ATOM	956	N	ASP	133	26.553	17.009	53.411	1.00	20.15	7
ATOM	957	CA	ASP	133	25.397	16.156	53.729	1.00	22.27	6
ATOM	958	CB	ASP	133	25.868	14.755	54.193	1.00	23.23	6
ATOM	959	CG	ASP	133	26.187	13.783	53.024	1.00	25.72	6
ATOM	960	OD1	ASP	133	25.704	14.012	51.871	1.00	26.91	8
ATOM	961	OD2	ASP	133	26.894	12.758	53.284	1.00	25.03	8
ATOM	962	C	ASP	133	24.655	16.814	54.885	1.00	22.10	6
ATOM	963	O	ASP	133	23.575	17.415	54.715	1.00	24.05	8
ATOM	964	N	GLU	134	25.310	16.802	56.037	1.00	19.91	7
ATOM	965	CA	GLU	134	24.742	17.410	57.211	1.00	18.60	6
ATOM	966	CB	GLU	134	25.478	16.953	58.482	1.00	17.36	6
ATOM	967	CG	GLU	134	26.589	15.897	58.287	1.00	17.83	6
ATOM	968	CD	GLU	134	28.003	16.514	58.153	1.00	20.37	6
ATOM	969	OE1	GLU	134	28.980	15.726	58.020	1.00	19.82	8
ATOM	970	OE2	GLU	134	28.136	17.775	58.183	1.00	18.81	8
ATOM	971	C	GLU	134	24.784	18.933	57.068	1.00	17.19	6
ATOM	972	O	GLU	134	25.842	19.534	57.197	1.00	18.37	8
ATOM	973	N	SER	135	23.648	19.496	56.657	1.00	16.42	7
ATOM	974	CA	SER	135	23.375	20.938	56.510	1.00	17.66	6
ATOM	975	CB	SER	135	24.435	21.857	57.166	1.00	17.67	6
ATOM	976	OG	SER	135	25.623	21.981	56.400	1.00	19.35	8
ATOM	977	C	SER	135	22.990	21.443	55.124	1.00	18.19	6
ATOM	978	O	SER	135	22.366	22.501	54.991	1.00	17.96	8
ATOM	979	N	GLY	136	23.287	20.665	54.095	1.00	19.82	7
ATOM	980	CA	GLY	136	22.945	21.109	52.753	1.00	21.54	6
ATOM	981	C	GLY	136	23.765	22.335	52.372	1.00	22.07	6
ATOM	982	O	GLY	136	23.225	23.345	51.910	1.00	22.69	8
ATOM	983	N	HIS	137	25.071	22.258	52.622	1.00	21.69	7
ATOM	984	CA	HIS	137	25.992	23.332	52.301	1.00	19.69	6
ATOM	985	CB	HIS	137	26.594	23.884	53.590	1.00	22.11	6
ATOM	986	CG	HIS	137	25.768	24.968	54.204	1.00	25.43	6
ATOM	987	CD2	HIS	137	26.049	25.862	55.183	1.00	27.18	6
ATOM	988	ND1	HIS	137	24.484	25.256	53.777	1.00	26.89	7
ATOM	989	CE1	HIS	137	24.014	26.287	54.465	1.00	26.67	6
ATOM	990	NE2	HIS	137	24.944	26.674	55.325	1.00	26.59	7
ATOM	991	C	HIS	137	27.081	22.863	51.329	1.00	19.46	6
ATOM	992	O	HIS	137	27.426	21.666	51.301	1.00	20.08	8
ATOM	993	N	VAL	138	27.547	23.771	50.468	1.00	16.09	7
ATOM	994	CA	VAL	138	28.598	23.427	49.526	1.00	12.40	6
ATOM	995	CB	VAL	138	28.391	24.107	48.143	1.00	12.43	6
ATOM	996	CG1	VAL	138	29.725	24.286	47.390	1.00	10.78	6
ATOM	997	CG2	VAL	138	27.444	23.258	47.290	1.00	12.93	6
ATOM	998	C	VAL	138	29.891	23.877	50.156	1.00	11.10	6
ATOM	999	O	VAL	138	29.960	24.976	50.705	1.00	11.62	8
ATOM	1000	N	VAL	139	30.872	22.982	50.171	1.00	9.36	7
ATOM	1001	CA	VAL	139	32.194	23.268	50.724	1.00	10.38	6
ATOM	1002	CB	VAL	139	32.539	22.371	51.949	1.00	6.78	6
ATOM	1003	CG1	VAL	139	33.781	22.877	52.620	1.00	7.80	6
ATOM	1004	CG2	VAL	139	31.415	22.393	52.946	1.00	6.80	6
ATOM	1005	C	VAL	139	33.249	23.095	49.615	1.00	10.04	6
ATOM	1006	O	VAL	139	33.333	22.026	49.961	1.00	10.34	8

bref21c.pdb Thu Apr 25 12:27:47 1996 14

ATOM	1007	N	LEU	140	33.975	24.194	49.372	1.00	8.25	7
ATOM	1008	CA	LEU	140	35.027	24.306	48.384	1.00	6.26	6
ATOM	1009	CB	LEU	140	34.986	25.673	47.761	1.00	2.05	6
ATOM	1010	CG	LEU	140	33.726	25.968	47.000	1.00	2.00	6
ATOM	1011	CD1	LEU	140	33.806	27.395	46.505	1.00	2.00	6
ATOM	1012	CD2	LEU	140	33.594	24.972	45.869	1.00	2.00	6
ATOM	1013	C	LEU	140	36.354	24.170	49.069	1.00	8.88	6
ATOM	1014	O	LEU	140	36.566	24.774	50.115	1.00	10.60	8
ATOM	1015	N	ARG	141	37.278	23.481	48.409	1.00	11.34	7
ATOM	1016	CA	ARG	141	38.618	23.235	48.929	1.00	12.76	6
ATOM	1017	CB	ARG	141	38.682	21.805	49.446	1.00	16.99	6
ATOM	1018	CG	ARG	141	39.347	21.645	50.793	1.00	21.35	6
ATOM	1019	CD	ARG	141	40.849	21.410	50.697	1.00	24.13	6
ATOM	1020	NE	ARG	141	41.431	21.433	52.042	1.00	29.12	7
ATOM	1021	CZ	ARG	141	42.344	22.314	52.462	1.00	30.00	6
ATOM	1022	NH1	ARG	141	42.821	23.266	51.673	1.00	30.75	7
ATOM	1023	NH2	ARG	141	42.727	22.282	53.773	1.00	29.95	7
ATOM	1024	C	ARG	141	39.632	23.383	47.804	1.00	13.10	6
ATOM	1025	O	ARG	141	39.289	23.227	46.639	1.00	13.55	8
ATOM	1026	N	TRP	142	40.871	23.715	48.154	1.00	11.10	7
ATOM	1027	CA	TRP	142	41.941	23.846	47.182	1.00	6.61	6
ATOM	1028	CB	TRP	142	41.754	25.107	46.354	1.00	6.92	6
ATOM	1029	CG	TRP	142	41.661	26.356	47.155	1.00	9.55	6
ATOM	1030	CD2	TRP	142	40.482	26.905	47.749	1.00	9.85	6
ATOM	1031	CE2	TRP	142	40.852	28.094	48.397	1.00	9.31	6
ATOM	1032	CE3	TRP	142	39.145	26.508	47.788	1.00	10.67	6
ATOM	1033	CD1	TRP	142	42.671	27.216	47.456	1.00	10.90	6
ATOM	1034	NE1	TRP	142	42.196	28.267	48.209	1.00	11.52	7
ATOM	1035	CZ2	TRP	142	39.937	28.885	49.072	1.00	11.31	6
ATOM	1036	CZ3	TRP	142	38.245	27.296	48.454	1.00	11.65	6
ATOM	1037	CH2	TRP	142	38.645	28.474	49.089	1.00	9.80	6
ATOM	1038	C	TRP	142	43.288	23.857	47.877	1.00	5.00	6
ATOM	1039	O	TRP	142	43.380	23.703	49.076	1.00	6.66	8
ATOM	1040	N	LEU	143	44.349	23.995	47.109	1.00	5.47	7
ATOM	1041	CA	LEU	143	45.700	24.039	47.656	1.00	3.56	6
ATOM	1042	CB	LEU	143	46.520	22.876	47.123	1.00	2.35	6
ATOM	1043	CG	LEU	143	46.031	21.474	47.408	1.00	2.00	6
ATOM	1044	CD1	LEU	143	46.832	20.483	46.601	1.00	2.00	6
ATOM	1045	CD2	LEU	143	46.182	21.223	48.862	1.00	2.00	6
ATOM	1046	C	LEU	143	46.310	25.326	47.158	1.00	2.00	6
ATOM	1047	O	LEU	143	45.765	25.970	46.274	1.00	4.81	8
ATOM	1048	N	PRO	144	47.411	25.759	47.762	1.00	2.00	7
ATOM	1049	CD	PRO	144	48.003	25.327	49.030	1.00	2.00	6
ATOM	1050	CA	PRO	144	48.027	26.996	47.295	1.00	2.00	6
ATOM	1051	CB	PRO	144	48.955	27.359	48.445	1.00	2.00	6
ATOM	1052	CG	PRO	144	48.442	26.605	49.601	1.00	2.00	6
ATOM	1053	C	PRO	144	48.821	26.750	46.011	1.00	2.00	6
ATOM	1054	O	PRO	144	48.999	25.611	45.580	1.00	2.00	8
ATOM	1055	N	PRO	145	49.249	27.823	45.342	1.00	2.00	7
ATOM	1056	CD	PRO	145	49.058	29.249	45.645	1.00	2.00	6
ATOM	1057	CA	PRO	145	50.022	27.643	44.113	1.00	2.72	6
ATOM	1058	CB	PRO	145	50.532	29.053	43.839	1.00	2.80	6
ATOM	1059	CG	PRO	145	49.467	29.898	44.372	1.00	2.95	6
ATOM	1060	C	PRO	145	51.178	26.696	44.455	1.00	4.71	6
ATOM	1061	O	PRO	145	51.875	26.899	45.448	1.00	3.80	8
ATOM	1062	N	PRO	146	51.396	25.652	43.639	1.00	8.22	7
ATOM	1063	CD	PRO	146	50.738	25.412	42.347	1.00	5.90	6
ATOM	1064	CA	PRO	146	52.462	24.665	43.857	1.00	6.83	6
ATOM	1065	CB	PRO	146	52.358	23.778	42.622	1.00	7.88	6
ATOM	1066	CG	PRO	146	50.972	23.951	42.167	1.00	6.28	6
ATOM	1067	C	PRO	146	53.863	25.273	43.967	1.00	9.28	6
ATOM	1068	O	PRO	146	54.272	26.087	43.135	1.00	10.56	8
ATOM	1069	N	GLU	147	54.604	24.825	44.975	1.00	10.54	7
ATOM	1070	CA	GLU	147	55.959	25.281	45.248	1.00	9.65	6
ATOM	1071	CB	GLU	147	56.894	24.958	44.077	1.00	9.95	6
ATOM	1072	CG	GLU	147	56.732	23.566	43.456	1.00	18.10	6
ATOM	1073	CD	GLU	147	57.477	22.401	44.166	1.00	22.76	6
ATOM	1074	OE1	GLU	147	58.335	22.639	45.061	1.00	26.12	8
ATOM	1075	OE2	GLU	147	57.207	21.215	43.789	1.00	23.73	8
ATOM	1076	C	GLU	147	56.052	26.773	45.624	1.00	10.12	6
ATOM	1077	O	GLU	147	57.099	27.408	45.453	1.00	12.66	8
ATOM	1078	N	THR	148	54.975	27.364	46.124	1.00	10.44	7
ATOM	1079	CA	THR	148	55.048	28.776	46.541	1.00	7.37	6
ATOM	1080	CB	THR	148	53.778	29.551	46.178	1.00	5.61	6
ATOM	1081	OG1	THR	148	52.589	28.464	44.765	1.00	4.74	8
ATOM	1082	CG2	THR	148	53.881	31.014	46.621	1.00	2.00	6
ATOM	1083	C	THR	148	55.272	28.818	48.048	1.00	6.00	6
ATOM	1084	O	THR	148	54.609	28.080	48.789	1.00	4.53	8

ATOM	1085	N	PRO	149	56.279	29.605	48.503	1.00	7.63	
ATOM	1086	CD	PRO	149	57.156	30.457	47.666	1.00	4.62	
ATOM	1087	CA	PRO	149	56.623	29.757	49.926	1.00	5.20	
ATOM	1088	CB	PRO	149	58.074	30.190	49.860	1.00	2.62	
ATOM	1089	CG	PRO	149	58.050	31.144	48.698	1.00	2.00	
ATOM	1090	C	PRO	149	55.742	30.869	50.498	1.00	7.00	
ATOM	1091	O	PRO	149	55.080	31.600	49.737	1.00	10.83	
ATOM	1092	N	MET	150	55.727	31.012	51.814	1.00	7.26	
ATOM	1093	CA	MET	150	54.916	32.048	52.464	1.00	5.41	
ATOM	1094	CB	MET	150	55.415	33.469	52.109	1.00	5.16	
ATOM	1095	CG	MET	150	56.864	33.812	52.512	1.00	2.00	
ATOM	1096	SD	MET	150	57.164	33.978	54.292	1.00	8.51	
ATOM	1097	CE	MET	150	57.009	35.706	54.546	1.00	2.48	
ATOM	1098	C	MET	150	53.411	31.927	52.169	1.00	5.15	
ATOM	1099	O	MET	150	52.749	32.952	52.002	1.00	4.08	
ATOM	1100	N	THR	151	52.878	30.696	52.239	1.00	3.72	
ATOM	1101	CA	THR	151	51.464	30.405	51.963	1.00	3.59	
ATOM	1102	CB	THR	151	51.157	28.902	51.799	1.00	2.22	
ATOM	1103	OG1	THR	151	51.581	28.183	52.955	1.00	8.69	
ATOM	1104	CG2	THR	151	51.821	28.347	50.609	1.00	3.84	
ATOM	1105	C	THR	151	50.403	30.920	52.922	1.00	5.68	
ATOM	1106	O	THR	151	49.218	30.919	52.583	1.00	7.24	
ATOM	1107	N	SER	152	50.774	31.331	54.123	1.00	6.42	
ATOM	1108	CA	SER	152	49.755	31.831	55.041	1.00	6.44	
ATOM	1109	CB	SER	152	50.178	31.598	56.476	1.00	6.46	
ATOM	1110	OG	SER	152	51.027	32.645	56.893	1.00	5.28	
ATOM	1111	C	SER	152	49.563	33.321	54.842	1.00	7.14	
ATOM	1112	O	SER	152	48.982	33.976	55.687	1.00	10.00	
ATOM	1113	N	HIS	153	50.148	33.866	53.780	1.00	7.23	
ATOM	1114	CA	HIS	153	50.070	35.291	53.485	1.00	5.69	
ATOM	1115	CB	HIS	153	51.479	35.883	53.275	1.00	4.92	
ATOM	1116	CG	HIS	153	52.310	35.975	54.526	1.00	4.89	
ATOM	1117	CD2	HIS	153	52.810	37.048	55.182	1.00	3.84	
ATOM	1118	ND1	HIS	153	52.781	34.868	55.197	1.00	6.02	
ATOM	1119	CE1	HIS	153	53.540	35.254	56.204	1.00	3.19	
ATOM	1120	NE2	HIS	153	53.573	36.570	56.215	1.00	2.00	
ATOM	1121	C	HIS	153	49.275	35.491	52.227	1.00	2.54	
ATOM	1122	O	HIS	153	49.013	36.614	51.811	1.00	6.78	
ATOM	1123	N	ILE	154	48.937	34.385	51.603	1.00	2.00	
ATOM	1124	CA	ILE	154	48.201	34.412	50.377	1.00	2.00	
ATOM	1125	CB	ILE	154	48.493	33.116	49.523	1.00	2.00	
ATOM	1126	CG2	ILE	154	47.906	33.208	48.126	1.00	2.06	
ATOM	1127	CG1	ILE	154	49.982	32.883	49.376	1.00	2.00	
ATOM	1128	CD1	ILE	154	50.301	31.727	48.512	1.00	2.00	
ATOM	1129	C	ILE	154	46.702	34.532	50.669	1.00	2.05	
ATOM	1130	O	ILE	154	46.165	33.897	51.564	1.00	2.00	
ATOM	1131	N	ARG	155	46.068	35.391	49.885	1.00	4.56	
ATOM	1132	CA	ARG	155	44.636	35.649	49.910	1.00	5.20	
ATOM	1133	CB	ARG	155	44.372	37.149	49.818	1.00	5.20	
ATOM	1134	CG	ARG	155	44.596	37.920	51.094	1.00	8.42	
ATOM	1135	CD	ARG	155	44.382	39.399	50.848	1.00	14.35	
ATOM	1136	NE	ARG	155	44.206	40.104	52.119	1.00	24.48	
ATOM	1137	CZ	ARG	155	44.832	41.229	52.496	1.00	27.35	
ATOM	1138	NH1	ARG	155	45.718	41.848	51.699	1.00	25.45	
ATOM	1139	NH2	ARG	155	44.600	41.707	53.725	1.00	28.94	
ATOM	1140	C	ARG	155	44.067	34.962	48.668	1.00	5.00	
ATOM	1141	O	ARG	155	44.800	34.760	47.678	1.00	5.22	
ATOM	1142	N	TYR	156	42.782	34.596	48.739	1.00	5.08	
ATOM	1143	CA	TYR	156	42.077	33.927	47.651	1.00	5.24	
ATOM	1144	CB	TYR	156	41.774	32.474	48.011	1.00	5.18	
ATOM	1145	CG	TYR	156	42.978	31.665	48.339	1.00	10.86	
ATOM	1146	CD1	TYR	156	43.447	31.591	49.651	1.00	13.49	
ATOM	1147	CE1	TYR	156	44.624	30.889	49.968	1.00	16.29	
ATOM	1148	CD2	TYR	156	43.700	31.012	47.341	1.00	14.47	
ATOM	1149	CE2	TYR	156	44.899	30.288	47.646	1.00	14.32	
ATOM	1150	CZ	TYR	156	45.346	30.240	48.960	1.00	14.29	
ATOM	1151	OH	TYR	156	46.495	29.567	49.289	1.00	12.88	
ATOM	1152	C	TYR	156	40.736	34.600	47.365	1.00	7.25	
ATOM	1153	O	TYR	156	40.151	35.204	48.256	1.00	8.19	
ATOM	1154	N	GLU	157	40.286	34.531	46.107	1.00	4.39	
ATOM	1155	CA	GLU	157	38.979	35.038	45.720	1.00	6.80	
ATOM	1156	CB	GLU	157	39.036	36.256	44.813	1.00	4.31	
ATOM	1157	CG	GLU	157	37.632	36.826	44.614	1.00	3.87	
ATOM	1158	CD	GLU	157	37.577	38.030	43.726	1.00	2.38	
ATOM	1159	OE1	GLU	157	37.568	39.171	44.232	1.00	4.23	
ATOM	1160	OE2	GLU	157	37.486	37.826	42.514	1.00	6.19	
ATOM	1161	C	GLU	157	38.254	33.920	44.997	1.00	6.19	
ATOM	1162	O	GLU	157	38.799	33.290	44.102	1.00	10.44	

bref21c.pdb Thu Apr 25 12:27:47 1996 16

ATOM	1163	N	VAL	158	37.022	33.675	45.406	1.00	5.40	
ATOM	1164	CA	VAL	158	36.196	32.627	44.842	1.00	6.15	
ATOM	1165	CB	VAL	158	35.459	31.877	45.954	1.00	3.03	
ATOM	1166	CG1	VAL	158	34.655	30.759	45.391	1.00	4.03	
ATOM	1167	CG2	VAL	158	36.429	31.369	46.962	1.00	3.63	
ATOM	1168	C	VAL	158	35.154	32.186	43.878	1.00	9.07	
ATOM	1169	O	VAL	158	34.400	34.103	44.208	1.00	10.93	
ATOM	1170	N	ASP	159	35.114	32.622	42.681	1.00	10.57	
ATOM	1171	CA	ASP	159	34.147	33.012	41.672	1.00	10.09	
ATOM	1172	CB	ASP	159	34.828	33.112	40.327	1.00	11.17	
ATOM	1173	CG	ASP	159	33.873	33.473	39.256	1.00	13.89	
ATOM	1174	OD1	ASP	159	33.863	32.822	38.172	1.00	13.65	
ATOM	1175	OD2	ASP	159	33.093	34.407	39.547	1.00	15.65	
ATOM	1176	C	ASP	159	32.997	31.985	41.575	1.00	9.91	
ATOM	1177	O	ASP	159	33.227	30.761	41.474	1.00	11.09	
ATOM	1178	N	VAL	160	31.766	32.485	41.627	1.00	7.83	
ATOM	1179	CA	VAL	160	30.582	31.642	41.535	1.00	5.49	
ATOM	1180	CB	VAL	160	29.637	31.774	42.755	1.00	3.19	
ATOM	1181	CG1	VAL	160	28.512	30.738	42.742	1.00	3.00	
ATOM	1182	CG2	VAL	160	30.362	31.602	44.091	1.00	2.00	
ATOM	1183	C	VAL	160	29.842	32.132	40.286	1.00	6.19	
ATOM	1184	O	VAL	160	29.364	33.280	40.238	1.00	8.22	
ATOM	1185	N	SER	161	29.835	31.272	39.300	1.00	7.72	
ATOM	1186	CA	SER	161	29.104	31.475	38.046	1.00	8.29	
ATOM	1187	CB	SER	161	30.094	31.628	36.891	1.00	10.26	
ATOM	1188	OG	SER	161	30.637	32.951	36.934	1.00	13.94	
ATOM	1189	C	SER	161	28.161	30.275	37.938	1.00	7.24	
ATOM	1190	O	SER	161	28.601	29.117	38.024	1.00	7.94	
ATOM	1191	N	ALA	162	26.885	30.605	37.791	1.00	9.16	
ATOM	1192	CA	ALA	162	25.793	29.612	37.784	1.00	12.39	
ATOM	1193	CB	ALA	162	24.689	30.055	38.736	1.00	15.24	
ATOM	1194	C	ALA	162	25.199	29.394	36.379	1.00	14.12	
ATOM	1195	O	ALA	162	25.593	30.044	35.406	1.00	13.91	
ATOM	1196	N	GLY	163	24.220	28.499	36.369	1.00	15.85	
ATOM	1197	CA	GLY	163	23.598	27.913	35.150	1.00	16.65	
ATOM	1198	C	GLY	163	22.561	28.761	34.370	1.00	18.26	
ATOM	1199	O	GLY	163	21.996	29.729	34.897	1.00	18.80	
ATOM	1200	N	ASN	164	22.416	28.231	33.146	1.00	90.00	
ATOM	1201	CA	ASN	164	21.568	28.664	31.994	1.00	90.00	
ATOM	1202	CB	ASN	164	20.505	27.625	31.685	1.00	90.00	
ATOM	1203	CG	ASN	164	19.337	27.730	32.702	1.00	90.00	
ATOM	1204	OD1	ASN	164	19.322	27.033	33.726	1.00	90.00	
ATOM	1205	ND2	ASN	164	18.334	28.580	32.511	1.00	90.00	
ATOM	1206	C	ASN	164	20.728	29.929	32.186	1.00	90.00	
ATOM	1207	O	ASN	164	19.665	29.874	32.817	1.00	90.00	
ATOM	1208	N	GLY	165	21.227	31.004	31.601	1.00	90.00	
ATOM	1209	CA	GLY	165	20.544	32.321	31.514	1.00	90.00	
ATOM	1210	C	GLY	165	20.274	33.048	32.859	1.00	90.00	
ATOM	1211	O	GLY	165	19.470	33.987	32.927	1.00	90.00	
ATOM	1212	N	ALA	166	20.941	32.706	33.967	1.00	90.00	
ATOM	1213	CA	ALA	166	20.602	33.406	35.242	1.00	90.00	
ATOM	1214	CB	ALA	166	19.550	32.609	36.015	1.00	90.00	
ATOM	1215	C	ALA	166	21.795	33.647	36.188	1.00	90.00	
ATOM	1216	O	ALA	166	21.646	33.653	37.421	1.00	90.00	
ATOM	1217	N	GLY	167	22.964	33.851	35.614	1.00	11.62	
ATOM	1218	CA	GLY	167	24.167	34.185	36.400	1.00	13.44	
ATOM	1219	C	GLY	167	24.110	35.688	36.704	1.00	15.68	
ATOM	1220	O	GLY	167	23.701	36.494	35.863	1.00	15.58	
ATOM	1221	N	SER	168	24.304	36.099	37.909	1.00	17.86	
ATOM	1222	CA	SER	168	24.434	37.545	38.252	1.00	18.83	
ATOM	1223	CB	SER	168	23.543	37.788	39.465	1.00	21.82	
ATOM	1224	OG	SER	168	22.556	38.750	39.118	1.00	22.47	
ATOM	1225	C	SER	168	25.820	38.200	38.537	1.00	18.61	
ATOM	1226	O	SER	168	25.961	39.425	38.506	1.00	18.81	
ATOM	1227	N	VAL	169	26.808	37.379	38.789	1.00	16.64	
ATOM	1228	CA	VAL	169	28.218	37.762	39.149	1.00	17.78	
ATOM	1229	CB	VAL	169	28.719	39.141	38.657	1.00	19.01	
ATOM	1230	CG1	VAL	169	30.262	39.261	38.769	1.00	16.57	
ATOM	1231	CG2	VAL	169	28.407	39.441	37.197	1.00	18.24	
ATOM	1232	C	VAL	169	28.387	37.796	40.666	1.00	17.25	
ATOM	1233	O	VAL	169	28.222	38.845	41.313	1.00	15.44	
ATOM	1234	N	GLN	170	28.725	36.631	41.201	1.00	15.91	
ATOM	1235	CA	GLN	170	28.905	36.476	42.647	1.00	17.12	
ATOM	1236	CB	GLN	170	27.928	35.459	43.231	1.00	19.39	
ATOM	1237	CG	GLN	170	27.921	35.468	44.766	1.00	24.35	
ATOM	1238	CD	GLN	170	28.202	34.091	45.365	1.00	26.34	
ATOM	1239	OE1	GLN	170	27.369	33.192	45.247	1.00	27.24	
ATOM	1240	NE2	GLN	170	29.335	33.862	46.004	1.00	28.12	

ATOM	1241	C	GLN	170	30.344	36.030	43.047	1.00	14.76	6
ATOM	1242	O	GLN	170	30.735	34.892	42.819	1.00	10.49	8
ATOM	1243	N	ARG	171	31.101	36.932	43.674	1.00	13.88	7
ATOM	1244	CA	ARG	171	32.477	36.643	44.094	1.00	13.53	6
ATOM	1245	CB	ARG	171	33.441	37.718	43.573	1.00	13.16	6
ATOM	1246	CG	ARG	171	33.545	37.814	42.049	1.00	12.56	6
ATOM	1247	CD	ARG	171	34.460	36.738	41.425	1.00	13.31	6
ATOM	1248	NE	ARG	171	34.628	36.922	39.969	1.00	10.48	7
ATOM	1249	CZ	ARG	171	35.274	37.932	39.376	1.00	8.84	6
ATOM	1250	NH1	ARG	171	35.841	38.899	40.105	1.00	4.37	7
ATOM	1251	NH2	ARG	171	35.304	38.000	38.045	1.00	6.87	7
ATOM	1252	C	ARG	171	32.581	36.543	45.630	1.00	15.23	6
ATOM	1253	O	ARG	171	31.706	37.062	46.350	1.00	17.57	8
ATOM	1254	N	VAL	172	33.651	35.916	46.131	1.00	11.99	7
ATOM	1255	CA	VAL	172	33.816	35.727	47.565	1.00	9.19	6
ATOM	1256	CB	VAL	172	33.473	34.260	48.000	1.00	10.74	6
ATOM	1257	CG1	VAL	172	33.300	34.155	49.521	1.00	5.41	6
ATOM	1258	CG2	VAL	172	32.236	33.745	47.262	1.00	11.43	6
ATOM	1259	C	VAL	172	35.216	35.966	48.031	1.00	9.92	6
ATOM	1260	O	VAL	172	36.134	35.398	47.507	1.00	10.28	8
ATOM	1261	N	GLU	173	35.365	36.778	49.062	1.00	14.35	7
ATOM	1262	CA	GLU	173	36.671	37.041	49.657	1.00	14.21	6
ATOM	1263	CB	GLU	173	36.760	38.463	50.218	1.00	17.07	6
ATOM	1264	CG	GLU	173	36.591	39.569	49.173	1.00	21.96	6
ATOM	1265	CD	GLU	173	37.267	40.903	49.573	1.00	25.14	6
ATOM	1266	OE1	GLU	173	37.709	41.647	48.649	1.00	23.21	8
ATOM	1267	OE2	GLU	173	37.359	41.206	50.803	1.00	26.88	8
ATOM	1268	C	GLU	173	36.910	36.016	50.779	1.00	13.64	6
ATOM	1269	O	GLU	173	36.017	35.720	51.592	1.00	13.24	8
ATOM	1270	N	ILE	174	38.087	35.403	50.719	1.00	14.30	7
ATOM	1271	CA	ILE	174	38.557	34.406	51.669	1.00	14.95	6
ATOM	1272	CB	ILE	174	38.915	33.088	50.966	1.00	12.11	6
ATOM	1273	CG2	ILE	174	40.014	32.388	51.689	1.00	13.06	6
ATOM	1274	CG1	ILE	174	37.679	32.182	50.893	1.00	13.75	6
ATOM	1275	CD1	ILE	174	36.625	32.629	49.917	1.00	12.34	6
ATOM	1276	C	ILE	174	39.802	35.051	52.250	1.00	15.60	6
ATOM	1277	O	ILE	174	40.563	35.693	51.532	1.00	17.19	8
ATOM	1278	N	LEU	175	39.982	34.956	53.558	1.00	16.67	7
ATOM	1279	CA	LEU	175	41.138	35.582	54.166	1.00	16.56	6
ATOM	1280	CB	LEU	175	40.838	35.972	55.609	1.00	15.47	6
ATOM	1281	CG	LEU	175	40.467	37.466	55.733	1.00	16.91	6
ATOM	1282	CD1	LEU	175	40.100	38.112	54.394	1.00	14.03	6
ATOM	1283	CD2	LEU	175	39.345	37.623	56.733	1.00	16.66	6
ATOM	1284	C	LEU	175	42.394	34.753	54.031	1.00	16.41	6
ATOM	1285	O	LEU	175	42.322	33.535	53.838	1.00	17.23	8
ATOM	1286	N	GLU	176	43.542	35.431	54.084	1.00	17.18	7
ATOM	1287	CA	GLU	176	44.842	34.765	53.946	1.00	16.66	6
ATOM	1288	CB	GLU	176	46.000	35.733	54.145	1.00	21.33	6
ATOM	1289	CG	GLU	176	45.963	36.472	55.432	1.00	20.62	6
ATOM	1290	CD	GLU	176	46.145	37.925	55.180	1.00	22.84	6
ATOM	1291	OE1	GLU	176	47.330	38.343	55.218	1.00	23.62	8
ATOM	1292	OE2	GLU	176	45.117	38.626	54.911	1.00	23.22	8
ATOM	1293	C	GLU	176	45.068	33.602	54.852	1.00	12.93	6
ATOM	1294	O	GLU	176	44.875	33.686	56.062	1.00	16.37	8
ATOM	1295	N	GLY	177	45.574	32.545	54.259	1.00	9.95	7
ATOM	1296	CA	GLY	177	45.839	31.341	55.001	1.00	8.11	6
ATOM	1297	C	GLY	177	44.738	30.340	54.827	1.00	7.43	6
ATOM	1298	O	GLY	177	44.990	29.169	54.962	1.00	9.00	8
ATOM	1299	N	ARG	178	43.536	30.787	54.493	1.00	7.50	7
ATOM	1300	CA	ARG	178	42.398	29.882	54.316	1.00	8.26	6
ATOM	1301	CB	ARG	178	41.116	30.660	54.477	1.00	10.81	6
ATOM	1302	CG	ARG	178	41.154	31.621	55.616	1.00	14.76	6
ATOM	1303	CD	ARG	178	40.911	30.920	56.950	1.00	20.12	6
ATOM	1304	NE	ARG	178	41.904	31.285	57.960	1.00	24.00	7
ATOM	1305	CZ	ARG	178	42.400	32.509	58.135	1.00	26.21	6
ATOM	1306	NH1	ARG	178	42.004	33.543	57.381	1.00	27.32	7
ATOM	1307	NH2	ARG	178	43.350	32.687	59.043	1.00	26.51	7
ATOM	1308	C	ARG	178	42.375	29.216	52.954	1.00	7.67	6
ATOM	1309	O	ARG	178	42.486	29.881	51.938	1.00	8.54	8
ATOM	1310	N	THR	179	42.205	27.906	52.934	1.00	7.97	7
ATOM	1311	CA	THR	179	42.148	27.157	51.689	1.00	9.51	6
ATOM	1312	CB	THR	179	43.376	26.310	51.542	1.00	9.72	6
ATOM	1313	OG1	THR	179	43.659	25.708	52.818	1.00	12.75	8
ATOM	1314	CG2	THR	179	44.559	27.162	51.073	1.00	6.02	6
ATOM	1315	C	THR	179	40.892	26.265	51.641	1.00	14.19	6
ATOM	1316	O	THR	179	40.892	25.102	51.155	1.00	15.46	8
ATOM	1317	N	GLU	180	39.770	26.831	52.151	1.00	13.36	7
ATOM	1318	CA	GLU	180	38.469	26.188	52.162	1.00	12.94	6

```
ATOM   1319  CB  GLU   180      38.329  25.242  53.340  1.00 14.42      6
ATOM   1320  CG  GLU   180      37.418  24.052  53.048  1.00 18.37      6
ATOM   1321  CD  GLU   180      37.112  23.255  54.299  1.00 19.86      6
ATOM   1322  OE1 GLU   180      36.526  23.877  55.216  1.00 21.31      8
ATOM   1323  OE2 GLU   180      37.473  22.045  54.387  1.00 18.58      8
ATOM   1324  C   GLU   180      37.442  27.288  52.301  1.00 14.56      6
ATOM   1325  O   GLU   180      37.742  28.385  52.782  1.00 14.76      8
ATOM   1326  N   CYS   181      36.209  26.986  51.934  1.00 13.82      7
ATOM   1327  CA  CYS   181      35.149  27.967  52.034  1.00 12.64      6
ATOM   1328  CB  CYS   181      35.382  28.990  50.936  1.00 12.66      6
ATOM   1329  SG  CYS   181      33.911  29.643  50.288  1.00 13.38     16
ATOM   1330  C   CYS   181      33.766  27.287  51.905  1.00 13.84      6
ATOM   1331  O   CYS   181      33.606  26.383  51.086  1.00 15.56      8
ATOM   1332  N   VAL   182      32.790  27.639  52.743  1.00 13.12      7
ATOM   1333  CA  VAL   182      31.478  26.985  52.613  1.00 11.97      6
ATOM   1334  CB  VAL   182      31.093  26.072  53.820  1.00  9.54      6
ATOM   1335  CG1 VAL   182      32.003  26.307  55.003  1.00 10.81      6
ATOM   1336  CG2 VAL   182      29.669  26.255  54.193  1.00  8.15      6
ATOM   1337  C   VAL   182      30.353  27.910  52.171  1.00 12.84      6
ATOM   1338  O   VAL   182      29.930  28.828  52.872  1.00 13.90      8
ATOM   1339  N   LEU   183      29.954  27.715  50.930  1.00 11.79      7
ATOM   1340  CA  LEU   183      28.921  28.515  50.338  1.00 12.76      6
ATOM   1341  CB  LEU   183      29.052  28.500  48.817  1.00 13.26      6
ATOM   1342  CG  LEU   183      30.193  29.380  48.350  1.00 11.81      6
ATOM   1343  CD1 LEU   183      30.636  28.956  46.970  1.00  8.24      6
ATOM   1344  CD2 LEU   183      29.734  30.852  48.398  1.00 13.01      6
ATOM   1345  C   LEU   183      27.566  28.027  50.778  1.00 14.24      6
ATOM   1346  O   LEU   183      27.139  26.887  50.514  1.00 15.09      8
ATOM   1347  N   SER   184      26.897  28.909  51.487  1.00 14.69      7
ATOM   1348  CA  SER   184      25.583  28.642  51.998  1.00 16.60      6
ATOM   1349  CB  SER   184      25.558  29.046  53.461  1.00 17.40      6
ATOM   1350  OG  SER   184      26.601  28.369  54.144  1.00 18.79      8
ATOM   1351  C   SER   184      24.671  29.537  51.208  1.00 17.61      6
ATOM   1352  O   SER   184      25.115  30.545  50.679  1.00 18.84      8
ATOM   1353  N   ASN   185      23.422  29.140  51.048  1.00 18.50      7
ATOM   1354  CA  ASN   185      22.479  29.998  50.338  1.00 21.04      6
ATOM   1355  CB  ASN   185      22.463  31.389  51.008  1.00 27.82      6
ATOM   1356  CG  ASN   185      22.274  31.330  52.546  1.00 33.52      6
ATOM   1357  OD1 ASN   185      22.899  32.131  53.270  1.00 36.61      8
ATOM   1358  ND2 ASN   185      21.392  30.414  53.050  1.00 36.25      7
ATOM   1359  C   ASN   185      22.641  30.149  48.794  1.00 19.48      6
ATOM   1360  O   ASN   185      22.967  31.228  48.263  1.00 18.46      8
ATOM   1361  N   LEU   186      22.329  29.062  48.093  1.00 17.53      7
ATOM   1362  CA  LEU   186      22.384  28.972  46.635  1.00 15.82      6
ATOM   1363  CB  LEU   186      23.632  28.170  46.201  1.00 14.99      6
ATOM   1364  CG  LEU   186      25.006  28.318  46.924  1.00 15.24      6
ATOM   1365  CD1 LEU   186      25.951  27.172  46.540  1.00 13.51      6
ATOM   1366  CD2 LEU   186      25.689  29.663  46.637  1.00 14.02      6
ATOM   1367  C   LEU   186      21.069  28.230  46.261  1.00 16.15      6
ATOM   1368  O   LEU   186      20.445  27.566  47.116  1.00 16.68      8
ATOM   1369  N   ARG   187      20.611  28.382  45.019  1.00 15.66      7
ATOM   1370  CA  ARG   187      19.371  27.749  44.576  1.00 14.27      6
ATOM   1371  CB  ARG   187      18.845  28.415  43.327  1.00 14.63      6
ATOM   1372  CG  ARG   187      19.152  29.870  43.263  1.00 19.73      6
ATOM   1373  CD  ARG   187      18.525  30.512  42.054  1.00 23.74      6
ATOM   1374  NE  ARG   187      19.218  30.197  40.905  1.00 26.90      7
ATOM   1375  CZ  ARG   187      18.997  29.109  40.060  1.00 28.07      6
ATOM   1376  NH1 ARG   187      18.110  28.181  40.430  1.00 29.72      7
ATOM   1377  NH2 ARG   187      19.594  29.001  38.874  1.00 31.36      7
ATOM   1378  C   ARG   187      19.528  26.264  44.298  1.00 16.07      6
ATOM   1379  O   ARG   187      20.608  25.788  43.872  1.00 14.20      8
ATOM   1380  N   GLY   188      18.413  25.557  44.483  1.00 15.94      7
ATOM   1381  CA  GLY   188      18.369  24.124  44.291  1.00 17.35      6
ATOM   1382  C   GLY   188      18.304  23.695  42.842  1.00 18.74      6
ATOM   1383  O   GLY   188      17.760  24.421  42.016  1.00 20.69      8
ATOM   1384  N   ARG   189      18.822  22.492  42.568  1.00 20.12      7
ATOM   1385  CA  ARG   189      18.891  21.885  41.239  1.00 20.15      6
ATOM   1386  CB  ARG   189      17.495  21.501  40.721  1.00 22.54      6
ATOM   1387  CG  ARG   189      17.450  20.203  39.871  1.00 26.04      6
ATOM   1388  CD  ARG   189      17.780  20.447  38.380  1.00 26.92      6
ATOM   1389  NE  ARG   189      18.570  19.373  37.756  1.00 27.40      7
ATOM   1390  CZ  ARG   189      18.076  18.215  37.299  1.00 29.60      6
ATOM   1391  NH1 ARG   189      16.768  17.933  37.405  1.00 30.45      7
ATOM   1392  NH2 ARG   189      18.888  17.342  36.686  1.00 28.39      7
ATOM   1393  C   ARG   189      19.610  22.773  41.218  1.00 20.12      6
ATOM   1394  O   ARG   189      19.406  22.605  38.317  1.00 21.60      8
ATOM   1395  N   THR   190      20.432  23.719  40.693  1.00 19.12      7
ATOM   1396  CA  THR   190      21.195  24.611  38.812  1.00 17.35      6
```

ATOM	1397	CB	THR	190	21.494	25.944	40.460	1.00	15.30	
ATOM	1398	OG1	THR	190	20.370	26.366	41.226	1.00	18.33	
ATOM	1399	CG2	THR	190	21.869	26.984	39.390	1.00	10.48	
ATOM	1400	C	THR	190	22.576	24.017	39.612	1.00	17.97	
ATOM	1401	O	THR	190	23.024	23.222	40.428	1.00	17.12	
ATOM	1402	N	ARG	191	23.262	24.460	38.563	1.00	18.62	
ATOM	1403	CA	ARG	191	24.621	24.018	38.253	1.00	18.64	
ATOM	1404	CB	ARG	191	24.783	23.686	36.746	1.00	23.05	
ATOM	1405	CG	ARG	191	26.243	23.477	36.278	1.00	28.15	
ATOM	1406	CD	ARG	191	26.802	22.032	36.502	1.00	29.37	
ATOM	1407	NE	ARG	191	26.824	21.206	35.274	1.00	31.41	
ATOM	1408	CZ	ARG	191	27.677	21.329	34.236	1.00	30.79	
ATOM	1409	NH1	ARG	191	28.650	22.261	34.198	1.00	30.54	
ATOM	1410	NH2	ARG	191	27.562	20.481	33.210	1.00	30.20	
ATOM	1411	C	ARG	191	25.471	25.213	38.627	1.00	15.56	
ATOM	1412	O	ARG	191	25.174	26.344	38.233	1.00	14.09	
ATOM	1413	N	TYR	192	26.495	24.950	39.417	1.00	12.55	
ATOM	1414	CA	TYR	192	27.380	25.971	39.901	1.00	11.03	
ATOM	1415	CB	TYR	192	27.283	26.027	41.411	1.00	10.18	
ATOM	1416	CG	TYR	192	26.063	26.759	41.890	1.00	13.18	
ATOM	1417	CD1	TYR	192	26.105	28.138	42.101	1.00	14.17	
ATOM	1418	CE1	TYR	192	24.949	28.867	42.435	1.00	14.60	
ATOM	1419	CD2	TYR	192	24.837	26.111	42.039	1.00	14.10	
ATOM	1420	CE2	TYR	192	23.670	26.840	42.371	1.00	15.93	
ATOM	1421	CZ	TYR	192	23.745	28.217	42.554	1.00	13.34	
ATOM	1422	OH	TYR	192	22.618	28.972	42.755	1.00	14.24	
ATOM	1423	C	TYR	192	28.759	25.557	39.508	1.00	12.33	
ATOM	1424	O	TYR	192	29.134	24.402	39.680	1.00	12.81	
ATOM	1425	N	THR	193	29.511	26.491	38.954	1.00	10.45	
ATOM	1426	CA	THR	193	30.875	26.230	38.535	1.00	7.07	
ATOM	1427	CB	THR	193	31.036	26.551	37.028	1.00	7.66	
ATOM	1428	OG1	THR	193	30.030	25.849	36.283	1.00	5.74	
ATOM	1429	CG2	THR	193	32.399	26.130	36.529	1.00	7.11	
ATOM	1430	C	THR	193	31.688	27.182	39.383	1.00	7.05	
ATOM	1431	O	THR	193	31.370	28.369	39.425	1.00	7.20	
ATOM	1432	N	PHE	194	32.685	26.682	40.113	1.00	8.39	
ATOM	1433	CA	PHE	194	33.487	27.571	40.967	1.00	5.90	
ATOM	1434	CB	PHE	194	33.421	27.133	42.427	1.00	6.97	
ATOM	1435	CG	PHE	194	32.030	26.778	42.900	1.00	8.68	
ATOM	1436	CD1	PHE	194	31.531	25.492	42.723	1.00	5.87	
ATOM	1437	CD2	PHE	194	31.222	27.735	43.519	1.00	8.15	
ATOM	1438	CE1	PHE	194	30.273	25.170	43.150	1.00	8.14	
ATOM	1439	CE2	PHE	194	29.957	27.412	43.946	1.00	5.23	
ATOM	1440	CZ	PHE	194	29.482	26.129	43.763	1.00	7.24	
ATOM	1441	C	PHE	194	34.922	27.565	40.524	1.00	5.55	
ATOM	1442	O	PHE	194	35.367	26.594	39.934	1.00	6.55	
ATOM	1443	N	ALA	195	35.646	28.633	40.849	1.00	5.34	
ATOM	1444	CA	ALA	195	37.057	28.785	40.494	1.00	4.57	
ATOM	1445	CB	ALA	195	37.173	29.298	39.047	1.00	5.31	
ATOM	1446	C	ALA	195	37.747	29.759	41.467	1.00	3.32	
ATOM	1447	O	ALA	195	37.101	30.692	41.921	1.00	2.79	
ATOM	1448	N	VAL	196	39.039	29.539	41.773	1.00	2.76	
ATOM	1449	CA	VAL	196	39.839	30.398	42.689	1.00	3.78	
ATOM	1450	CB	VAL	196	40.522	29.609	43.869	1.00	2.00	
ATOM	1451	CG1	VAL	196	40.237	30.276	45.214	1.00	2.00	
ATOM	1452	CG2	VAL	196	40.117	28.173	43.869	1.00	4.04	
ATOM	1453	C	VAL	196	41.000	31.085	41.995	1.00	2.07	
ATOM	1454	O	VAL	196	41.418	30.661	40.931	1.00	5.97	
ATOM	1455	N	ARG	197	41.531	32.121	42.629	1.00	2.00	
ATOM	1456	CA	ARG	197	42.687	32.860	42.129	1.00	2.00	
ATOM	1457	CB	ARG	197	42.279	33.902	41.069	1.00	2.00	
ATOM	1458	CG	ARG	197	41.384	35.010	41.574	1.00	2.00	
ATOM	1459	CD	ARG	197	41.062	36.000	40.504	1.00	2.00	
ATOM	1460	NE	ARG	197	40.345	37.124	41.073	1.00	3.47	
ATOM	1461	CZ	ARG	197	40.269	38.323	40.517	1.00	2.00	
ATOM	1462	NH1	ARG	197	40.846	38.550	39.357	1.00	2.00	
ATOM	1463	NH2	ARG	197	39.763	39.339	41.193	1.00	4.02	
ATOM	1464	C	ARG	197	43.374	33.489	43.362	1.00	2.09	
ATOM	1465	O	ARG	197	42.685	33.926	44.280	1.00	3.19	
ATOM	1466	N	ALA	198	44.710	33.490	43.399	1.00	2.00	
ATOM	1467	CA	ALA	198	45.475	33.996	44.550	1.00	2.47	
ATOM	1468	CB	ALA	198	46.420	32.903	45.072	1.00	2.30	
ATOM	1469	C	ALA	198	46.241	35.326	44.442	1.00	5.39	
ATOM	1470	O	ALA	198	46.614	35.772	43.340	1.00	2.19	
ATOM	1471	N	ARG	199	46.542	35.901	45.612	1.00	3.72	
ATOM	1472	CA	ARG	199	47.250	37.171	45.694	1.00	3.38	
ATOM	1473	CB	ARG	199	46.226	38.304	45.572	1.00	2.00	
ATOM	1474	CG	ARG	199	46.784	39.669	45.270	1.00	6.67	

bref21c.pdb Thu Apr 25 12:27:47 1996 20

ATOM	1475	CD	ARG	199	45.938	40.737	45.915	1.00	9.17	6
ATOM	1476	NE	ARG	199	46.306	42.120	45.579	1.00	13.78	7
ATOM	1477	CZ	ARG	199	46.187	42.662	44.363	1.00	15.94	6
ATOM	1478	NH1	ARG	199	45.738	41.950	43.329	1.00	18.32	7
ATOM	1479	NH2	ARG	199	46.417	43.954	44.181	1.00	18.45	7
ATOM	1480	C	ARG	199	48.030	37.321	47.023	1.00	5.53	6
ATOM	1481	O	ARG	199	47.555	36.916	48.058	1.00	8.08	8
ATOM	1482	N	MET	200	49.243	37.864	46.984	1.00	5.53	7
ATOM	1483	CA	MET	200	50.015	38.096	48.197	1.00	4.85	6
ATOM	1484	CB	MET	200	51.484	38.423	47.891	1.00	3.73	6
ATOM	1485	CG	MET	200	52.311	37.271	47.346	1.00	4.67	6
ATOM	1486	SD	MET	200	53.261	36.286	48.538	1.00	9.73	16
ATOM	1487	CE	MET	200	52.284	34.975	48.812	1.00	2.41	6
ATOM	1488	C	MET	200	49.340	39.289	48.874	1.00	7.02	6
ATOM	1489	O	MET	200	49.074	40.314	48.228	1.00	6.42	8
ATOM	1490	N	ALA	201	49.050	39.126	50.167	1.00	7.96	7
ATOM	1491	CA	ALA	201	48.369	40.140	50.962	1.00	10.65	6
ATOM	1492	CB	ALA	201	47.633	39.474	52.117	1.00	4.85	6
ATOM	1493	C	ALA	201	49.261	41.285	51.464	1.00	12.36	6
ATOM	1494	O	ALA	201	50.488	41.204	51.453	1.00	13.02	8
ATOM	1495	N	GLU	202	48.622	42.360	51.901	1.00	15.72	7
ATOM	1496	CA	GLU	202	49.336	43.527	52.421	1.00	19.04	6
ATOM	1497	CB	GLU	202	48.428	44.756	52.276	1.00	23.13	6
ATOM	1498	CG	GLU	202	47.650	44.796	50.914	1.00	28.94	6
ATOM	1499	CD	GLU	202	48.360	45.575	49.757	1.00	31.22	6
ATOM	1500	OE1	GLU	202	49.466	46.164	49.968	1.00	32.80	8
ATOM	1501	OE2	GLU	202	47.774	45.613	48.634	1.00	30.41	8
ATOM	1502	C	GLU	202	49.785	43.317	53.903	1.00	19.11	6
ATOM	1503	O	GLU	202	49.394	42.327	54.561	1.00	20.41	8
ATOM	1504	N	PRO	203	50.696	44.173	54.411	1.00	16.25	7
ATOM	1505	CD	PRO	203	51.150	44.143	55.820	1.00	15.32	6
ATOM	1506	CA	PRO	203	51.322	45.290	53.714	1.00	14.26	6
ATOM	1507	CB	PRO	203	51.339	46.367	54.782	1.00	13.02	6
ATOM	1508	CG	PRO	203	51.846	45.538	55.984	1.00	16.38	6
ATOM	1509	C	PRO	203	52.740	44.892	53.356	1.00	12.03	6
ATOM	1510	O	PRO	203	53.537	45.743	52.985	1.00	15.28	8
ATOM	1511	N	SER	204	53.073	43.623	53.540	1.00	8.98	7
ATOM	1512	CA	SER	204	54.420	43.146	53.222	1.00	11.79	6
ATOM	1513	CB	SER	204	54.674	41.764	53.868	1.00	11.87	6
ATOM	1514	OG	SER	204	55.093	41.856	55.224	1.00	12.48	8
ATOM	1515	C	SER	204	54.686	43.060	51.696	1.00	11.88	6
ATOM	1516	O	SER	204	55.632	43.660	51.152	1.00	11.24	8
ATOM	1517	N	PHE	205	53.818	42.309	51.031	1.00	10.89	7
ATOM	1518	CA	PHE	205	53.901	42.074	49.624	1.00	8.76	6
ATOM	1519	CB	PHE	205	53.911	40.573	49.390	1.00	8.70	6
ATOM	1520	CG	PHE	205	55.073	39.862	50.052	1.00	12.81	6
ATOM	1521	CD1	PHE	205	54.854	38.885	51.029	1.00	11.19	6
ATOM	1522	CD2	PHE	205	56.388	40.136	49.668	1.00	11.00	6
ATOM	1523	CE1	PHE	205	55.921	38.198	51.599	1.00	7.25	6
ATOM	1524	CE2	PHE	205	57.452	39.449	50.237	1.00	11.11	6
ATOM	1525	CZ	PHE	205	57.215	38.480	51.202	1.00	8.98	6
ATOM	1526	C	PHE	205	52.743	42.728	48.900	1.00	8.87	6
ATOM	1527	O	PHE	205	51.756	43.147	49.508	1.00	9.29	8
ATOM	1528	N	GLY	206	52.913	42.864	47.592	1.00	8.57	7
ATOM	1529	CA	GLY	206	51.892	43.459	46.751	1.00	8.14	6
ATOM	1530	C	GLY	206	52.007	42.855	45.367	1.00	7.24	6
ATOM	1531	O	GLY	206	52.956	42.124	45.081	1.00	8.58	8
ATOM	1532	N	GLY	207	51.020	43.080	44.520	1.00	7.18	7
ATOM	1533	CA	GLY	207	51.122	42.534	43.176	1.00	7.59	6
ATOM	1534	C	GLY	207	49.825	42.355	42.430	1.00	4.80	6
ATOM	1535	O	GLY	207	48.857	43.048	42.656	1.00	5.05	8
ATOM	1536	N	PHE	208	49.784	41.332	41.608	1.00	3.71	7
ATOM	1537	CA	PHE	208	48.621	41.069	40.805	1.00	3.73	6
ATOM	1538	CB	PHE	208	49.034	41.071	39.322	1.00	6.46	6
ATOM	1539	CG	PHE	208	50.158	42.013	39.011	1.00	6.53	6
ATOM	1540	CD1	PHE	208	49.956	43.377	39.004	1.00	6.75	6
ATOM	1541	CD2	PHE	208	51.441	41.530	38.793	1.00	9.68	6
ATOM	1542	CE1	PHE	208	51.022	44.253	38.790	1.00	7.99	6
ATOM	1543	CE2	PHE	208	52.506	42.393	38.579	1.00	8.12	6
ATOM	1544	CZ	PHE	208	52.292	43.756	38.580	1.00	6.95	6
ATOM	1545	C	PHE	208	47.896	39.767	41.149	1.00	2.21	6
ATOM	1546	O	PHE	208	48.463	38.823	41.704	1.00	2.77	8
ATOM	1547	N	TRP	209	46.602	39.780	40.878	1.00	2.30	7
ATOM	1548	CA	TRP	209	45.766	38.625	41.073	1.00	3.71	6
ATOM	1549	CB	TRP	209	44.302	38.979	40.811	1.00	4.79	6
ATOM	1550	CG	TRP	209	43.505	39.378	42.011	1.00	4.76	6
ATOM	1551	CD2	TRP	209	43.156	38.550	43.104	1.00	2.67	6
ATOM	1552	CE2	TRP	209	42.347	39.316	43.959	1.00	2.87	6

ATOM	1553	CE3	TRP	209	43.445	37.234	43.446	1.00	2.00	
ATOM	1554	CD1	TRP	209	42.908	40.586	42.240	1.00	2.25	
ATOM	1555	NE1	TRP	209	42.211	40.554	43.396	1.00	2.00	
ATOM	1556	CZ2	TRP	209	41.825	36.809	45.148	1.00	4.70	
ATOM	1557	CZ3	TRP	209	42.933	36.729	44.616	1.00	4.57	
ATOM	1558	CH2	TRP	209	42.131	37.513	45.461	1.00	4.76	
ATOM	1559	C	TRP	209	46.222	37.604	40.033	1.00	3.17	
ATOM	1560	O	TRP	209	46.556	37.969	38.920	1.00	3.26	
ATOM	1561	N	SER	210	46.235	36.335	40.412	1.00	4.99	
ATOM	1562	CA	SER	210	46.650	35.269	39.533	1.00	5.26	
ATOM	1563	CB	SER	210	46.903	34.002	40.337	1.00	4.60	
ATOM	1564	OG	SER	210	45.683	33.363	40.660	1.00	3.40	
ATOM	1565	C	SER	210	45.571	34.968	38.515	1.00	9.26	
ATOM	1566	O	SER	210	44.564	35.689	38.398	1.00	13.86	
ATOM	1567	N	ALA	211	45.832	33.924	37.735	1.00	10.41	
ATOM	1568	CA	ALA	211	44.895	33.423	36.757	1.00	10.30	
ATOM	1569	CB	ALA	211	45.639	32.571	35.768	1.00	10.37	
ATOM	1570	C	ALA	211	43.893	32.558	37.567	1.00	11.25	
ATOM	1571	O	ALA	211	44.160	32.175	38.706	1.00	14.78	
ATOM	1572	N	TRP	212	42.736	32.263	37.014	1.00	9.47	
ATOM	1573	CA	TRP	212	41.791	31.433	37.734	1.00	7.74	
ATOM	1574	CB	TRP	212	40.447	31.434	36.993	1.00	9.05	
ATOM	1575	CG	TRP	212	39.723	32.765	36.942	1.00	4.98	
ATOM	1576	CD2	TRP	212	39.061	33.399	38.030	1.00	2.00	
ATOM	1577	CE2	TRP	212	38.529	34.597	37.547	1.00	2.33	
ATOM	1578	CE3	TRP	212	38.867	33.063	39.367	1.00	2.00	
ATOM	1579	CD1	TRP	212	39.566	33.576	35.867	1.00	2.00	
ATOM	1580	NE1	TRP	212	38.850	34.680	36.219	1.00	2.00	
ATOM	1581	CZ2	TRP	212	37.811	35.470	38.359	1.00	4.55	
ATOM	1582	CZ3	TRP	212	38.162	33.921	40.167	1.00	2.47	
ATOM	1583	CH2	TRP	212	37.640	35.111	39.671	1.00	2.13	
ATOM	1584	C	TRP	212	42.340	30.012	37.771	1.00	8.93	
ATOM	1585	O	TRP	212	43.262	29.696	37.043	1.00	8.63	
ATOM	1586	N	SER	213	41.771	29.145	38.598	1.00	11.16	
ATOM	1587	CA	SER	213	42.222	27.747	38.642	1.00	11.60	
ATOM	1588	CB	SER	213	42.041	27.183	40.045	1.00	12.78	
ATOM	1589	OG	SER	213	40.667	27.131	40.397	1.00	13.18	
ATOM	1590	C	SER	213	41.303	26.959	37.738	1.00	12.67	
ATOM	1591	O	SER	213	40.265	27.471	37.293	1.00	14.82	
ATOM	1592	N	GLU	214	41.644	25.718	37.441	1.00	12.59	
ATOM	1593	CA	GLU	214	40.694	24.971	36.660	1.00	12.29	
ATOM	1594	CB	GLU	214	41.307	23.662	36.198	1.00	16.37	
ATOM	1595	CG	GLU	214	42.107	23.797	34.873	1.00	23.12	
ATOM	1596	CD	GLU	214	41.249	24.291	33.640	1.00	27.82	
ATOM	1597	OE1	GLU	214	41.627	25.337	33.001	1.00	29.07	
ATOM	1598	OE2	GLU	214	40.218	23.631	33.301	1.00	27.91	
ATOM	1599	C	GLU	214	39.550	24.814	37.680	1.00	11.57	
ATOM	1600	O	GLU	214	39.793	24.625	38.864	1.00	11.86	
ATOM	1601	N	PRO	215	38.301	25.037	37.258	1.00	11.02	
ATOM	1602	CD	PRO	215	37.959	25.363	35.868	1.00	12.93	
ATOM	1603	CA	PRO	215	37.068	24.965	38.059	1.00	11.49	
ATOM	1604	CB	PRO	215	36.155	25.896	37.290	1.00	9.49	
ATOM	1605	CG	PRO	215	36.430	25.447	35.937	1.00	12.12	
ATOM	1606	C	PRO	215	36.378	23.609	38.237	1.00	9.78	
ATOM	1607	O	PRO	215	36.664	22.654	37.525	1.00	12.44	
ATOM	1608	N	VAL	216	35.440	22.553	38.172	1.00	7.47	
ATOM	1609	CA	VAL	216	34.669	22.346	39.434	1.00	7.05	
ATOM	1610	CB	VAL	216	34.740	21.829	40.924	1.00	8.24	
ATOM	1611	CG1	VAL	216	35.569	20.568	41.016	1.00	9.46	
ATOM	1612	CG2	VAL	216	35.226	22.929	41.918	1.00	6.68	
ATOM	1613	C	VAL	216	33.261	22.834	39.259	1.00	9.31	
ATOM	1614	O	VAL	216	33.001	24.039	39.445	1.00	10.20	
ATOM	1615	N	SER	217	32.357	21.913	38.937	1.00	8.47	
ATOM	1616	CA	SER	217	30.952	22.247	38.766	1.00	9.61	
ATOM	1617	CB	SER	217	30.549	22.157	37.302	1.00	10.53	
ATOM	1618	OG	SER	217	29.610	23.179	37.004	1.00	13.22	
ATOM	1619	C	SER	217	30.127	21.282	39.601	1.00	10.91	
ATOM	1620	O	SER	217	30.424	20.086	39.647	1.00	9.60	
ATOM	1621	N	LEU	218	29.067	21.791	40.224	1.00	10.82	
ATOM	1622	CA	LEU	218	28.223	20.981	41.102	1.00	11.10	
ATOM	1623	CB	LEU	218	28.605	21.295	42.566	1.00	9.62	
ATOM	1624	CG	LEU	218	27.995	20.615	43.789	1.00	6.92	
ATOM	1625	CD1	LEU	218	28.207	19.150	43.686	1.00	9.37	
ATOM	1626	CD2	LEU	218	28.647	21.135	45.053	1.00	8.78	
ATOM	1627	C	LEU	218	26.727	21.208	40.903	1.00	12.91	
ATOM	1628	O	LEU	218	26.306	22.335	40.693	1.00	12.22	
ATOM	1629	N	LEU	219	25.958	20.114	40.670	1.00	14.15	
ATOM	1630	CA	LEU	219	24.486	20.164	40.760	1.00	13.92	

```
bref21c.pdb          Thu Apr 25 12:27:47 1996        22

ATOM   1631  CB  LEU   219      23.867  18.372  40.209  1.00 13.95      6
ATOM   1632  CG  LEU   219      23.819  18.429  38.736  1.00 16.57      6
ATOM   1633  CD1 LEU   219      22.857  19.308  37.947  1.00 18.05      6
ATOM   1634  CD2 LEU   219      25.208  18.810  38.096  1.00 15.67      6
ATOM   1635  C   LEU   219      24.080  20.226  42.248  1.00 12.96      6
ATOM   1636  O   LEU   219      24.378  19.295  42.986  1.00 12.64      8
ATOM   1637  N   THR   220      23.501  21.329  42.692  1.00 12.52      7
ATOM   1638  CA  THR   220      23.057  21.472  44.068  1.00 10.27      6
ATOM   1639  CB  THR   220      22.289  22.744  44.250  1.00 10.52      6
ATOM   1640  OG1 THR   220      22.030  23.330  42.967  1.00 14.44      8
ATOM   1641  CG2 THR   220      23.076  23.704  45.099  1.00 13.55      6
ATOM   1642  C   THR   220      22.111  20.325  44.368  1.00 11.61      6
ATOM   1643  O   THR   220      21.196  20.053  43.582  1.00 13.03      8
ATOM   1644  N   THR   303      67.975  42.384  64.372  1.00 11.41      7
ATOM   1645  CA  THR   303      67.750  41.604  65.597  1.00  9.49      6
ATOM   1646  CB  THR   303      66.400  42.008  66.344  1.00 10.05      6
ATOM   1647  OG1 THR   303      65.988  43.329  65.963  1.00 12.85      8
ATOM   1648  CG2 THR   303      66.595  42.033  67.861  1.00 12.80      6
ATOM   1649  C   THR   303      67.737  40.103  65.280  1.00  9.93      6
ATOM   1650  O   THR   303      68.525  39.342  65.838  1.00  9.37      8
ATOM   1651  N   TYR   304      66.882  39.690  64.343  1.00 10.17      7
ATOM   1652  CA  TYR   304      66.756  38.281  63.973  1.00  9.53      6
ATOM   1653  CB  TYR   304      65.306  37.826  64.148  1.00  7.06      6
ATOM   1654  CG  TYR   304      64.839  37.837  65.585  1.00  7.97      6
ATOM   1655  CD1 TYR   304      64.311  39.130  66.072  1.00  4.80      6
ATOM   1656  CE1 TYR   304      64.003  39.268  67.389  1.00  3.80      6
ATOM   1657  CD2 TYR   304      65.030  36.680  66.486  1.00  6.93      6
ATOM   1658  CE2 TYR   304      64.721  37.015  67.809  1.00  4.43      6
ATOM   1659  CZ  TYR   304      64.208  38.221  68.261  1.00  4.88      6
ATOM   1660  OH  TYR   304      63.886  38.359  69.598  1.00 10.24      8
ATOM   1661  C   TYR   304      67.182  38.065  62.554  1.00  8.23      6
ATOM   1662  O   TYR   304      67.277  39.024  61.804  1.00 11.69      8
ATOM   1663  N   SER   305      67.474  36.819  62.201  1.00  8.34      7
ATOM   1664  CA  SER   305      67.856  36.442  60.843  1.00  9.43      6
ATOM   1665  CB  SER   305      69.204  35.705  60.838  1.00 13.12      6
ATOM   1666  OG  SER   305      70.226  36.516  61.427  1.00 18.03      8
ATOM   1667  C   SER   305      66.736  35.557  60.273  1.00 10.05      6
ATOM   1668  O   SER   305      66.490  34.433  60.754  1.00 10.34      8
ATOM   1669  N   CYS   306      66.093  36.051  59.218  1.00  8.05      7
ATOM   1670  CA  CYS   306      64.968  35.364  58.619  1.00  5.52      6
ATOM   1671  C   CYS   306      64.970  35.039  57.131  1.00  6.70      6
ATOM   1672  O   CYS   306      65.609  35.702  56.302  1.00  6.69      8
ATOM   1673  CB  CYS   306      63.738  36.288  58.889  1.00  6.36      6
ATOM   1674  SG  CYS   306      63.703  36.826  60.556  1.00  8.87     16
ATOM   1675  N   HIS   307      64.186  34.026  56.808  1.00  6.09      7
ATOM   1676  CA  HIS   307      64.015  33.604  55.459  1.00  7.50      6
ATOM   1677  CB  HIS   307      65.038  32.519  55.083  1.00 11.44      6
ATOM   1678  CG  HIS   307      64.853  31.183  55.746  1.00 14.32      6
ATOM   1679  CD2 HIS   307      64.068  30.124  55.420  1.00 16.07      6
ATOM   1680  ND1 HIS   307      65.706  30.728  56.734  1.00 16.54      7
ATOM   1681  CE1 HIS   307      65.467  29.468  56.976  1.00 14.82      6
ATOM   1682  NE2 HIS   307      64.478  29.056  56.192  1.00 17.24      7
ATOM   1683  C   HIS   307      62.576  33.176  55.236  1.00  9.06      6
ATOM   1684  O   HIS   307      61.811  32.990  56.188  1.00 11.93      8
ATOM   1685  N   PHE   308      62.167  33.136  53.980  1.00  8.50      7
ATOM   1686  CA  PHE   308      60.815  32.725  53.647  1.00  6.83      6
ATOM   1687  CB  PHE   308      60.481  33.092  52.167  1.00  7.92      6
ATOM   1688  CG  PHE   308      60.530  34.557  51.891  1.00  5.48      6
ATOM   1689  CD1 PHE   308      61.140  35.016  50.747  1.00  6.64      6
ATOM   1690  CD2 PHE   308      59.935  35.482  52.738  1.00  9.42      6
ATOM   1691  CE1 PHE   308      61.152  36.402  50.448  1.00  8.48      6
ATOM   1692  CE2 PHE   308      59.942  36.871  52.445  1.00  9.15      6
ATOM   1693  CZ  PHE   308      60.547  37.324  51.307  1.00  6.33      6
ATOM   1694  C   PHE   308      60.689  31.207  53.849  1.00  5.44      6
ATOM   1695  O   PHE   308      61.489  30.434  53.322  1.00  4.17      8
ATOM   1696  N   GLY   309      59.746  30.803  54.691  1.00  5.25      7
ATOM   1697  CA  GLY   309      59.517  29.391  54.922  1.00  5.83      6
ATOM   1698  C   GLY   309      58.315  28.874  54.098  1.00  6.57      6
ATOM   1699  O   GLY   309      57.806  29.566  53.316  1.00  8.19      8
ATOM   1700  N   PRO   310      57.791  27.756  54.223  1.00  5.60      7
ATOM   1701  CD  PRO   310      58.486  26.582  54.742  1.00  3.04      6
ATOM   1702  CA  PRO   310      56.648  27.419  53.364  1.00  5.55      6
ATOM   1703  CB  PRO   310      56.581  25.887  53.449  1.00  3.33      6
ATOM   1704  CG  PRO   310      57.956  25.497  53.857  1.00 10.25      6
ATOM   1705  C   PRO   310      55.395  28.077  53.909  1.00  9.52      6
ATOM   1706  O   PRO   310      54.387  28.241  53.139  1.00 12.37      8
ATOM   1707  N   LEU   311      55.322  28.503  55.161  1.00  6.38      7
ATOM   1708  CA  LEU   311      54.145  29.114  55.756  1.00  5.58      6
```

ATOM	1709	CB	LEU	311	53.834	28.437	57.080	1.00	4.94
ATOM	1710	CG	LEU	311	52.837	27.277	57.127	1.00	5.34
ATOM	1711	CD1	LEU	311	51.524	27.802	57.619	1.00	5.36
ATOM	1712	CD2	LEU	311	52.684	26.580	55.781	1.00	5.32
ATOM	1713	C	LEU	311	54.346	30.580	56.002	1.00	4.95
ATOM	1714	O	LEU	311	53.586	31.411	55.540	1.00	4.76
ATOM	1715	N	THR	312	55.390	30.898	56.741	1.00	5.31
ATOM	1716	CA	THR	312	55.680	32.285	57.075	1.00	7.62
ATOM	1717	CB	THR	312	54.772	32.732	58.256	1.00	7.52
ATOM	1718	OG1	THR	312	54.898	34.144	58.476	1.00	10.56
ATOM	1719	CG2	THR	312	55.115	31.951	59.526	1.00	6.36
ATOM	1720	C	THR	312	57.168	32.342	57.444	1.00	6.58
ATOM	1721	O	THR	312	57.868	31.352	57.215	1.00	7.15
ATOM	1722	N	TRP	313	57.641	33.477	57.979	1.00	5.96
ATOM	1723	CA	TRP	313	59.050	33.653	58.382	1.00	6.02
ATOM	1724	CB	TRP	313	59.294	35.032	58.992	1.00	5.13
ATOM	1725	CG	TRP	313	58.937	36.213	58.158	1.00	5.28
ATOM	1726	CD2	TRP	313	59.685	36.779	57.066	1.00	6.34
ATOM	1727	CE2	TRP	313	59.026	37.968	56.682	1.00	4.38
ATOM	1728	CE3	TRP	313	60.845	36.403	56.382	1.00	8.66
ATOM	1729	CD1	TRP	313	57.883	37.044	58.359	1.00	4.69
ATOM	1730	NE1	TRP	313	57.933	38.103	57.488	1.00	5.50
ATOM	1731	CZ2	TRP	313	59.484	38.784	55.656	1.00	4.75
ATOM	1732	CZ3	TRP	313	61.301	37.222	55.350	1.00	6.62
ATOM	1733	CH2	TRP	313	60.618	38.398	55.004	1.00	5.72
ATOM	1734	C	TRP	313	59.605	32.619	59.389	1.00	8.38
ATOM	1735	O	TRP	313	58.931	32.186	60.359	1.00	9.40
ATOM	1736	N	VAL	314	60.847	32.216	59.139	1.00	7.40
ATOM	1737	CA	VAL	314	61.533	31.286	60.013	1.00	6.87
ATOM	1738	CB	VAL	314	62.145	30.110	59.249	1.00	4.82
ATOM	1739	CG1	VAL	314	62.868	29.204	60.190	1.00	9.24
ATOM	1740	CG2	VAL	314	61.099	29.333	58.536	1.00	3.95
ATOM	1741	C	VAL	314	62.637	32.192	60.499	1.00	8.62
ATOM	1742	O	VAL	314	63.512	32.562	59.730	1.00	11.83
ATOM	1743	N	CYS	315	62.516	32.672	61.724	1.00	9.61
ATOM	1744	CA	CYS	315	63.524	33.567	62.250	1.00	10.57
ATOM	1745	C	CYS	315	64.417	32.948	63.293	1.00	10.10
ATOM	1746	O	CYS	315	64.191	31.825	63.748	1.00	11.89
ATOM	1747	CB	CYS	315	62.905	34.861	62.757	1.00	10.52
ATOM	1748	SG	CYS	315	62.176	35.824	61.399	1.00	7.84
ATOM	1749	N	LYS	316	65.402	33.724	63.715	1.00	10.83
ATOM	1750	CA	LYS	316	66.381	33.242	64.650	1.00	9.93
ATOM	1751	CB	LYS	316	67.301	32.320	63.860	1.00	10.47
ATOM	1752	CG	LYS	316	68.200	31.444	64.637	1.00	12.32
ATOM	1753	CD	LYS	316	69.242	30.818	63.708	1.00	13.72
ATOM	1754	CE	LYS	316	70.213	31.865	63.178	1.00	17.21
ATOM	1755	NZ	LYS	316	71.029	32.467	64.288	1.00	17.34
ATOM	1756	C	LYS	316	67.141	34.462	65.092	1.00	11.52
ATOM	1757	O	LYS	316	67.193	35.468	64.359	1.00	9.91
ATOM	1758	N	PRO	317	67.592	34.516	66.355	1.00	9.25
ATOM	1759	CD	PRO	317	67.284	33.617	67.471	1.00	7.88
ATOM	1760	CA	PRO	317	68.344	35.662	66.855	1.00	10.51
ATOM	1761	CB	PRO	317	68.365	35.412	68.348	1.00	8.33
ATOM	1762	CG	PRO	317	68.381	33.979	68.426	1.00	6.27
ATOM	1763	C	PRO	317	69.773	35.714	66.285	1.00	14.13
ATOM	1764	O	PRO	317	70.533	34.732	66.339	1.00	14.85
ATOM	1765	N	GLN	318	70.105	36.867	65.711	1.00	16.42
ATOM	1766	CA	GLN	318	71.418	37.137	65.144	1.00	16.93
ATOM	1767	CB	GLN	318	71.369	38.436	64.326	1.00	15.12
ATOM	1768	CG	GLN	318	72.010	38.335	62.946	1.00	16.24
ATOM	1769	CD	GLN	318	71.602	39.482	62.064	1.00	17.29
ATOM	1770	OE1	GLN	318	70.734	39.341	61.189	1.00	15.50
ATOM	1771	NE2	GLN	318	72.199	40.642	62.305	1.00	16.42
ATOM	1772	C	GLN	318	72.273	37.386	66.360	1.00	16.25
ATOM	1773	O	GLN	318	71.906	38.227	67.174	1.00	15.24
ATOM	1774	N	THR	403	70.252	35.791	66.614	1.00	11.35
ATOM	1775	CA	THR	403	69.393	36.058	54.455	1.00	12.98
ATOM	1776	CB	THR	403	68.236	34.931	54.252	1.00	14.68
ATOM	1777	OG1	THR	403	68.911	33.658	54.627	1.00	14.88
ATOM	1778	CG2	THR	403	67.869	34.883	52.748	1.00	12.39
ATOM	1779	C	THR	403	66.757	37.471	54.551	1.00	11.13
ATOM	1780	O	THR	403	69.149	38.341	53.757	1.00	11.39
ATOM	1781	N	TYR	404	67.778	37.693	55.454	1.00	8.66
ATOM	1782	CA	TYR	404	67.195	39.040	55.682	1.00	8.10
ATOM	1783	CB	TYR	404	65.698	39.119	55.366	1.00	8.26
ATOM	1784	CG	TYR	404	65.333	38.966	53.910	1.00	8.42
ATOM	1785	CD1	TYR	404	65.036	37.707	53.377	1.00	8.78
ATOM	1786	CE1	TYR	404	64.723	37.548	52.042	1.00	8.00

bref21c.pdb Thu Apr 25 12:27:47 1996 24

```
ATOM   1787  CD2 TYR   404      65.299  40.071  53.050  1.00  2.00
ATOM   1788  CE2 TYR   404      64.992  39.918  51.710  1.00  2.00
ATOM   1789  CZ  TYR   404      64.709  38.650  51.219  1.00  2.53
ATOM   1790  OH  TYR   404      64.447  38.463  49.891  1.00  6.21
ATOM   1791  C   TYR   404      67.374  39.373  57.169  1.00  6.87
ATOM   1792  O   TYR   404      67.459  38.477  58.006  1.00  5.71
ATOM   1793  N   SER   405      67.453  40.653  57.500  1.00  7.44
ATOM   1794  CA  SER   405      67.581  41.068  58.894  1.00  7.96
ATOM   1795  CB  SER   405      68.842  41.887  59.094  1.00  9.81
ATOM   1796  OG  SER   405      69.985  41.082  58.888  1.00 14.61
ATOM   1797  C   SER   405      66.332  41.863  59.305  1.00 10.09
ATOM   1798  O   SER   405      66.154  43.047  58.975  1.00 10.03
ATOM   1799  N   CYS   406      65.466  41.198  60.046  1.00 10.45
ATOM   1800  CA  CYS   406      64.220  41.789  60.452  1.00 10.00
ATOM   1801  C   CYS   406      64.192  42.035  61.938  1.00 10.98
ATOM   1802  O   CYS   406      64.900  41.386  62.709  1.00 12.25
ATOM   1803  CB  CYS   406      63.096  40.827  60.107  1.00 12.32
ATOM   1804  SG  CYS   406      63.277  39.951  58.514  1.00 12.21
ATOM   1805  N   HIS   407      63.363  42.987  62.332  1.00 10.98
ATOM   1806  CA  HIS   407      63.162  43.317  63.721  1.00  8.89
ATOM   1807  CB  HIS   407      64.007  44.542  64.165  1.00 11.52
ATOM   1808  CG  HIS   407      63.779  45.803  63.370  1.00 12.77
ATOM   1809  CD2 HIS   407      64.324  46.233  62.204  1.00 11.11
ATOM   1810  ND1 HIS   407      62.968  46.832  63.812  1.00 10.97
ATOM   1811  CE1 HIS   407      63.025  47.837  62.954  1.00 10.32
ATOM   1812  NE2 HIS   407      63.840  47.499  61.969  1.00 10.00
ATOM   1813  C   HIS   407      61.687  43.614  63.801  1.00  3.26
ATOM   1814  O   HIS   407      61.078  43.935  62.789  1.00 10.54
ATOM   1815  N   PHE   408      61.099  43.443  64.976  1.00  7.42
ATOM   1816  CA  PHE   408      59.690  43.746  65.168  1.00  6.36
ATOM   1817  CB  PHE   408      59.281  43.636  66.643  1.00  5.63
ATOM   1818  CG  PHE   408      59.441  42.280  67.218  1.00  3.30
ATOM   1819  CD1 PHE   408      59.675  42.125  68.562  1.00  4.11
ATOM   1820  CD2 PHE   408      59.411  41.158  66.409  1.00  4.22
ATOM   1821  CE1 PHE   408      59.888  40.882  69.095  1.00  2.80
ATOM   1822  CE2 PHE   408      59.626  39.885  66.935  1.00  4.80
ATOM   1823  CZ  PHE   408      59.866  39.751  68.282  1.00  4.71
ATOM   1824  C   PHE   408      59.459  45.185  64.736  1.00  6.02
ATOM   1825  O   PHE   408      60.370  46.018  64.744  1.00  8.84
ATOM   1826  N   GLY   409      58.231  45.463  64.347  1.00  4.91
ATOM   1827  CA  GLY   409      57.868  46.791  63.936  1.00  2.33
ATOM   1828  C   GLY   409      56.494  46.954  64.509  1.00  2.02
ATOM   1829  O   GLY   409      55.996  46.065  65.196  1.00  4.33
ATOM   1830  N   PRO   410      55.879  48.100  64.299  1.00  2.00
ATOM   1831  CD  PRO   410      56.497  49.286  63.693  1.00  2.98
ATOM   1832  CA  PRO   410      54.544  48.397  64.788  1.00  3.72
ATOM   1833  CB  PRO   410      54.276  49.754  64.166  1.00  6.67
ATOM   1834  CG  PRO   410      55.622  50.390  64.195  1.00  6.29
ATOM   1835  C   PRO   410      53.525  47.367  64.313  1.00  7.04
ATOM   1836  O   PRO   410      52.831  46.752  65.137  1.00  8.58
ATOM   1837  N   LEU   411      53.471  47.165  62.987  1.00  6.97
ATOM   1838  CA  LEU   411      52.544  46.233  62.328  1.00  5.66
ATOM   1839  CB  LEU   411      52.254  46.674  60.898  1.00  8.28
ATOM   1840  CG  LEU   411      51.310  47.803  60.553  1.00 11.17
ATOM   1841  CD1 LEU   411      50.007  47.519  61.244  1.00 15.07
ATOM   1842  CD2 LEU   411      51.886  49.156  60.961  1.00 14.05
ATOM   1843  C   LEU   411      53.052  44.831  62.192  1.00  4.04
ATOM   1844  O   LEU   411      52.365  43.870  62.481  1.00  2.78
ATOM   1845  N   THR   412      54.237  44.705  61.643  1.00  3.16
ATOM   1846  CA  THR   412      54.749  43.388  61.431  1.00  2.09
ATOM   1847  CB  THR   412      52.985  42.829  60.244  1.00  2.00
ATOM   1848  OG1 THR   412      54.152  41.413  60.166  1.00  4.84
ATOM   1849  CG2 THR   412      54.417  43.523  58.976  1.00  2.00
ATOM   1850  C   THR   412      56.252  43.565  61.220  1.00  2.54
ATOM   1851  O   THR   412      56.722  44.675  61.376  1.00  3.32
ATOM   1852  N   TRP   413      57.003  42.490  60.964  1.00  3.36
ATOM   1853  CA  TRP   413      58.468  42.579  60.747  1.00  4.26
ATOM   1854  CB  TRP   413      59.003  41.293  60.115  1.00  3.65
ATOM   1855  CG  TRP   413      58.912  40.078  60.909  1.00  2.26
ATOM   1856  CD2 TRP   413      59.722  39.724  62.023  1.00  4.36
ATOM   1857  CE2 TRP   413      59.374  38.418  62.398  1.00  3.99
ATOM   1858  CE3 TRP   413      60.712  40.409  62.745  1.00  5.87
ATOM   1859  CD1 TRP   413      58.121  39.011  60.667  1.00  2.00
ATOM   1860  NE1 TRP   413      58.395  37.998  61.546  1.00  3.14
ATOM   1861  CZ2 TRP   413      59.975  37.766  63.459  1.00  7.15
ATOM   1862  CZ3 TRP   413      61.312  39.764  63.801  1.00  7.66
ATOM   1863  CH2 TRP   413      60.941  38.451  64.152  1.00  9.17
ATOM   1864  C   TRP   413      58.960  43.720  59.832  1.00  2.50
```

```
ATOM  1865  C   TRP   413      58.187  44.350  59.115  1.00  7.06      6
ATOM  1866  N   VAL   414      60.272  43.923  59.813  1.00  6.50      6
ATOM  1867  CA  VAL   414      60.904  44.921  58.957  1.00  6.63      6
ATOM  1868  CB  VAL   414      61.078  46.289  59.660  1.00  7.88      6
ATOM  1869  CG1 VAL   414      62.193  47.072  59.029  1.00  6.76      6
ATOM  1870  CG2 VAL   414      59.789  47.111  59.547  1.00  8.37      6
ATOM  1871  C   VAL   414      62.242  44.340  58.533  1.00  9.59      6
ATOM  1872  O   VAL   414      63.183  44.296  59.303  1.00 11.73      8
ATOM  1873  N   CYS   415      62.296  43.820  57.314  1.00  9.75      7
ATOM  1874  CA  CYS   415      63.518  43.222  56.809  1.00  9.19      6
ATOM  1875  C   CYS   415      64.238  44.007  55.767  1.00  9.05      6
ATOM  1876  O   CYS   415      63.714  44.949  55.189  1.00  8.76      8
ATOM  1877  CB  CYS   415      63.207  41.882  56.222  1.00  9.11      6
ATOM  1878  SG  CYS   415      62.067  41.071  57.341  1.00 14.13     16
ATOM  1879  N   LYS   416      65.484  43.622  55.581  1.00  7.88      7
ATOM  1880  CA  LYS   416      66.341  44.197  54.585  1.00  9.50      6
ATOM  1881  CB  LYS   416      67.176  45.349  55.135  1.00 14.71      6
ATOM  1882  CG  LYS   416      66.482  46.235  56.144  1.00 19.54      6
ATOM  1883  CD  LYS   416      66.618  45.629  57.541  1.00 23.24      6
ATOM  1884  CE  LYS   416      65.851  46.404  58.599  1.00 23.74      6
ATOM  1885  NZ  LYS   416      66.292  45.888  59.937  1.00 27.08      7
ATOM  1886  C   LYS   416      67.234  43.008  54.278  1.00 12.10      6
ATOM  1887  O   LYS   416      67.523  42.187  55.175  1.00 10.95      8
ATOM  1888  N   PRO   417      67.578  42.817  52.990  1.00 12.45      7
ATOM  1889  CD  PRO   417      67.231  43.561  51.771  1.00 11.38      6
ATOM  1890  CA  PRO   417      66.434  41.684  52.671  1.00 11.76      6
ATOM  1891  CB  PRO   417      68.394  41.647  51.144  1.00 10.58      6
ATOM  1892  CG  PRO   417      68.247  43.047  50.780  1.00 11.41      6
ATOM  1893  C   PRO   417      69.845  41.868  53.221  1.00 14.43      6
ATOM  1894  O   PRO   417      70.361  42.990  53.325  1.00 14.95      8
ATOM  1895  N   GLN   418      70.400  40.762  53.700  1.00 15.69      7
ATOM  1896  CA  GLN   418      71.753  40.741  54.209  1.00 16.01      6
ATOM  1897  CB  GLN   418      71.933  39.562  55.165  1.00 15.85      6
ATOM  1898  CG  GLN   418      71.948  39.963  56.620  1.00 13.51      6
ATOM  1899  CD  GLN   418      71.580  38.823  57.530  1.00 16.21      6
ATOM  1900  OE1 GLN   418      71.377  37.668  57.098  1.00 16.54      8
ATOM  1901  NE2 GLN   418      71.478  39.131  58.807  1.00 16.18      7
ATOM  1902  C   GLN   418      72.660  40.583  52.990  1.00 17.91      6
ATOM  1903  O   GLN   418      72.470  39.656  52.172  1.00 20.26      8
ATOM  1904  N   LYS   510      36.636  45.747  96.455  1.00 20.08      7
ATOM  1905  CA  LYS   510      36.983  44.827  97.554  1.00 22.39      6
ATOM  1906  CB  LYS   510      37.004  45.503  98.958  1.00 22.50      6
ATOM  1907  CG  LYS   510      37.794  44.729 100.099  1.00 24.41      6
ATOM  1908  CD  LYS   510      39.382  44.786  99.984  1.00 24.33      6
ATOM  1909  CE  LYS   510      40.149  44.388 101.309  1.00 25.09      6
ATOM  1910  NZ  LYS   510      40.281  42.907 101.710  1.00 21.46      7
ATOM  1911  C   LYS   510      36.039  43.642  97.542  1.00 21.11      6
ATOM  1912  O   LYS   510      36.217  42.777  99.413  1.00 20.71      8
ATOM  1913  N   PHE   511      35.089  43.650  96.604  1.00 20.62      7
ATOM  1914  CA  PHE   511      34.207  42.501  96.453  1.00 18.81      6
ATOM  1915  CB  PHE   511      32.903  42.833  95.720  1.00 17.03      6
ATOM  1916  CG  PHE   511      31.969  41.646  95.592  1.00 17.36      6
ATOM  1917  CD1 PHE   511      32.470  40.353  95.362  1.00 17.10      6
ATOM  1918  CD2 PHE   511      30.594  41.806  95.735  1.00 19.23      6
ATOM  1919  CE1 PHE   511      31.630  39.235  95.279  1.00 16.04      6
ATOM  1920  CE2 PHE   511      29.738  40.690  95.653  1.00 20.47      6
ATOM  1921  CZ  PHE   511      30.271  39.394  95.424  1.00 17.16      6
ATOM  1922  C   PHE   511      35.064  41.629  95.554  1.00 17.52      6
ATOM  1923  O   PHE   511      35.406  40.483  95.913  1.00 16.93      8
ATOM  1924  N   GLU   512      35.416  42.200  94.392  1.00 17.14      7
ATOM  1925  CA  GLU   512      36.244  41.509  93.406  1.00 18.20      6
ATOM  1926  CB  GLU   512      36.536  42.391  92.172  1.00 20.73      6
ATOM  1927  CG  GLU   512      37.496  41.754  91.075  1.00 28.00      6
ATOM  1928  CD  GLU   512      36.851  40.687  90.101  1.00 30.11      6
ATOM  1929  OE1 GLU   512      37.346  40.507  88.936  1.00 29.86      8
ATOM  1930  OE2 GLU   512      35.869  40.011  90.501  1.00 30.27      8
ATOM  1931  C   GLU   512      37.507  41.181  94.162  1.00 15.96      6
ATOM  1932  O   GLU   512      37.938  40.029  94.161  1.00 16.76      8
ATOM  1933  N   SER   513      37.984  42.163  94.930  1.00 12.17      7
ATOM  1934  CA  SER   513      39.184  42.009  95.745  1.00 12.13      6
ATOM  1935  CB  SER   513      39.534  43.314  96.443  1.00 12.70      6
ATOM  1936  OG  SER   513      40.319  43.054  97.594  1.00 13.07      8
ATOM  1937  C   SER   513      39.122  40.871  96.775  1.00 12.52      6
ATOM  1938  O   SER   513      40.041  40.023  96.846  1.00 14.35      8
ATOM  1939  N   LYS   514      38.056  40.844  97.573  1.00 11.94      7
ATOM  1940  CA  LYS   514      37.903  39.792  98.568  1.00  9.95      6
ATOM  1941  CB  LYS   514      36.839  40.121  99.605  1.00  7.59      6
ATOM  1942  CG  LYS   514      37.258  41.165 100.627  1.00  5.11      6
```

bref21c.pdb Thu Apr 25 12:27:47 1996 26

ATOM	1943	CD	LYS	514	36.388	41.093	101.842	1.00	2.00
ATOM	1944	CE	LYS	514	36.374	42.393	102.539	1.00	2.00
ATOM	1945	NZ	LYS	514	35.665	42.215	103.798	1.00	3.28
ATOM	1946	C	LYS	514	37.621	36.443	97.959	1.00	11.59
ATOM	1947	O	LYS	514	37.841	37.435	98.620	1.00	13.26
ATOM	1948	N	ALA	515	37.128	36.401	96.716	1.00	10.50
ATOM	1949	CA	ALA	515	36.876	37.117	96.036	1.00	9.26
ATOM	1950	CB	ALA	515	36.187	37.366	94.719	1.00	10.99
ATOM	1951	C	ALA	515	38.165	36.299	95.806	1.00	8.83
ATOM	1952	O	ALA	515	38.170	35.068	95.920	1.00	7.78
ATOM	1953	N	ALA	516	39.241	37.026	95.494	1.00	8.76
ATOM	1954	CA	ALA	516	40.562	36.478	95.204	1.00	7.65
ATOM	1955	CB	ALA	516	41.457	37.533	94.614	1.00	6.46
ATOM	1956	C	ALA	516	41.205	35.872	96.419	1.00	7.97
ATOM	1957	O	ALA	516	41.690	34.751	96.353	1.00	8.85
ATOM	1958	N	LEU	517	41.226	36.599	97.530	1.00	8.04
ATOM	1959	CA	LEU	517	41.809	36.040	98.743	1.00	5.52
ATOM	1960	CB	LEU	517	41.445	36.874	99.947	1.00	3.15
ATOM	1961	CG	LEU	517	42.141	38.193	100.158	1.00	4.53
ATOM	1962	CD1	LEU	517	41.717	39.177	99.108	1.00	3.66
ATOM	1963	CD2	LEU	517	41.754	38.683	101.519	1.00	4.29
ATOM	1964	C	LEU	517	41.271	34.634	98.992	1.00	7.39
ATOM	1965	O	LEU	517	42.009	33.751	99.437	1.00	10.93
ATOM	1966	N	LEU	518	39.997	34.433	98.648	1.00	8.49
ATOM	1967	CA	LEU	518	39.297	33.177	98.857	1.00	7.25
ATOM	1968	CB	LEU	518	37.845	33.467	99.273	1.00	5.35
ATOM	1969	CG	LEU	518	37.614	33.731	100.773	1.00	5.58
ATOM	1970	CD1	LEU	518	36.802	34.965	100.936	1.00	3.48
ATOM	1971	CD2	LEU	518	36.951	32.519	101.495	1.00	6.87
ATOM	1972	C	LEU	518	39.339	32.158	97.723	1.00	9.11
ATOM	1973	O	LEU	518	39.185	30.955	97.979	1.00	8.10
ATOM	1974	N	ALA	519	39.557	32.623	96.505	1.00	11.23
ATOM	1975	CA	ALA	519	39.603	31.726	95.342	1.00	13.55
ATOM	1976	CB	ALA	519	39.310	32.481	94.072	1.00	12.76
ATOM	1977	C	ALA	519	40.908	30.949	95.209	1.00	15.14
ATOM	1978	O	ALA	519	41.733	31.215	94.311	1.00	15.55
ATOM	1979	N	ALA	520	41.047	29.935	96.068	1.00	17.93
ATOM	1980	CA	ALA	520	42.228	29.064	96.115	1.00	19.81
ATOM	1981	CB	ALA	520	42.169	28.165	97.371	1.00	20.83
ATOM	1982	C	ALA	520	42.579	28.212	94.865	1.00	19.53
ATOM	1983	O	ALA	520	41.764	27.430	94.339	1.00	19.39
ATOM	1984	N	ARG	521	43.834	28.352	94.449	1.00	90.00
ATOM	1985	CA	ARG	521	44.407	27.633	93.322	1.00	90.00
ATOM	1986	CB	ARG	521	45.499	28.484	92.652	1.00	90.00
ATOM	1987	CG	ARG	521	45.117	29.950	92.441	1.00	90.00
ATOM	1988	CD	ARG	521	45.751	30.871	93.500	1.00	90.00
ATOM	1989	NE	ARG	521	45.512	30.373	94.854	1.00	90.00
ATOM	1990	CZ	ARG	521	46.279	29.452	95.464	1.00	90.00
ATOM	1991	NH1	ARG	521	47.251	28.957	94.843	1.00	90.00
ATOM	1992	NH2	ARG	521	45.888	28.889	96.620	1.00	90.00
ATOM	1993	C	ARG	521	45.018	26.343	93.866	1.00	90.00
ATOM	1994	O	ARG	521	44.842	26.022	95.032	1.00	90.00
ATOM	1995	N	GLY	522	45.710	25.592	93.022	1.00	90.00
ATOM	1996	CA	GLY	522	46.338	24.375	93.500	1.00	90.00
ATOM	1997	C	GLY	522	47.851	24.578	93.549	1.00	90.00
ATOM	1998	O	GLY	522	48.288	25.677	93.891	1.00	90.00
ATOM	1999	N	PRO	523	48.672	23.533	93.225	1.00	90.00
ATOM	2000	CD	PRO	523	48.070	22.203	92.929	1.00	90.00
ATOM	2001	CA	PRO	523	50.157	23.469	93.185	1.00	90.00
ATOM	2002	CB	PRO	523	50.429	22.304	92.201	1.00	90.00
ATOM	2003	CG	PRO	523	49.277	21.315	92.486	1.00	90.00
ATOM	2004	C	PRO	523	50.966	24.731	92.741	1.00	90.00
ATOM	2005	O	PRO	523	50.499	25.617	91.984	1.00	90.00
ATOM	2006	N	GLU	524	52.222	24.761	93.180	1.00	24.71
ATOM	2007	CA	GLU	524	53.121	25.851	92.829	1.00	23.43
ATOM	2008	CB	GLU	524	54.289	25.979	93.857	1.00	27.67
ATOM	2009	CG	GLU	524	55.487	24.958	93.730	1.00	29.29
ATOM	2010	CD	GLU	524	55.207	23.507	94.250	1.00	31.85
ATOM	2011	OE1	GLU	524	54.910	22.603	93.413	1.00	29.10
ATOM	2012	OE2	GLU	524	55.263	23.263	95.484	1.00	27.26
ATOM	2013	C	GLU	524	53.672	25.532	91.428	1.00	21.32
ATOM	2014	O	GLU	524	53.705	24.359	91.016	1.00	20.22
ATOM	2015	N	GLU	525	54.169	26.564	90.747	1.00	18.30
ATOM	2016	CA	GLU	525	54.722	26.411	89.427	1.00	18.85
ATOM	2017	CB	GLU	525	53.557	26.336	88.442	1.00	18.52
ATOM	2018	CG	GLU	525	53.857	25.563	87.149	1.00	27.12
ATOM	2019	CD	GLU	525	52.595	25.163	86.357	1.00	31.84
ATOM	2020	OE1	GLU	525	52.474	23.956	85.991	1.00	33.25

ATOM	2021	OE2	GLU	525	51.731	26.066	65.119	1.00	34.53	
ATOM	2022	C	GLU	525	55.572	27.633	89.150	1.00	8.91	
ATOM	2023	O	GLU	525	55.306	28.676	69.733	1.00	9.70	
ATOM	2024	N	LEU	526	56.619	27.495	88.331	1.00	5.52	
ATOM	2025	CA	LEU	526	57.455	28.638	87.940	1.00	4.14	
ATOM	2026	CB	LEU	526	58.859	28.182	87.485	1.00	4.80	
ATOM	2027	CG	LEU	526	60.103	29.082	87.590	1.00	2.00	
ATOM	2028	CD1	LEU	526	61.166	28.507	86.706	1.00	2.00	
ATOM	2029	CD2	LEU	526	59.856	30.499	87.193	1.00	2.00	
ATOM	2030	C	LEU	526	56.688	29.248	86.751	1.00	2.64	
ATOM	2031	O	LEU	526	56.527	28.607	85.733	1.00	2.80	
ATOM	2032	N	LEU	527	56.209	30.474	86.892	1.00	2.00	
ATOM	2033	CA	LEU	527	55.415	31.107	85.854	1.00	2.00	
ATOM	2034	CB	LEU	527	54.115	31.638	86.441	1.00	4.05	
ATOM	2035	CG	LEU	527	53.035	30.653	86.824	1.00	2.65	
ATOM	2036	CD1	LEU	527	51.951	31.429	87.441	1.00	2.00	
ATOM	2037	CD2	LEU	527	52.547	29.889	85.620	1.00	2.00	
ATOM	2038	C	LEU	527	56.110	32.256	85.176	1.00	4.04	
ATOM	2039	O	LEU	527	56.413	33.252	85.836	1.00	5.30	
ATOM	2040	N	CYS	528	56.234	32.176	83.844	1.00	3.62	
ATOM	2041	CA	CYS	528	56.929	33.199	83.051	1.00	2.97	
ATOM	2042	C	CYS	528	55.987	33.810	82.044	1.00	2.18	
ATOM	2043	O	CYS	528	55.087	33.127	81.560	1.00	2.61	
ATOM	2044	CB	CYS	528	58.132	32.593	82.282	1.00	2.00	
ATOM	2045	SG	CYS	528	59.491	31.832	83.234	1.00	2.00	
ATOM	2046	N	PHE	529	56.197	35.088	81.743	1.00	2.00	
ATOM	2047	CA	PHE	529	55.397	35.792	80.758	1.00	4.16	
ATOM	2048	CB	PHE	529	54.008	36.143	81.303	1.00	3.88	
ATOM	2049	CG	PHE	529	53.980	37.315	82.231	1.00	2.00	
ATOM	2050	CD1	PHE	529	53.958	38.611	81.733	1.00	2.00	
ATOM	2051	CD2	PHE	529	53.912	37.123	83.611	1.00	2.00	
ATOM	2052	CE1	PHE	529	53.868	39.697	82.590	1.00	2.00	
ATOM	2053	CE2	PHE	529	53.822	38.207	84.471	1.00	2.00	
ATOM	2054	CZ	PHE	529	53.801	39.490	83.961	1.00	2.00	
ATOM	2055	C	PHE	529	56.100	37.031	80.200	1.00	5.77	
ATOM	2056	O	PHE	529	57.078	37.511	80.785	1.00	6.52	
ATOM	2057	N	THR	530	55.665	37.471	79.018	1.00	2.84	
ATOM	2058	CA	THR	530	56.225	38.655	78.377	1.00	2.00	
ATOM	2059	CB	THR	530	57.228	38.280	77.232	1.00	2.00	
ATOM	2060	OG1	THR	530	57.683	39.460	76.579	1.00	2.84	
ATOM	2061	CG2	THR	530	56.637	37.355	76.234	1.00	2.96	
ATOM	2062	C	THR	530	55.076	39.582	77.948	1.00	2.59	
ATOM	2063	O	THR	530	53.999	39.124	77.611	1.00	4.31	
ATOM	2064	N	GLU	531	55.275	40.882	78.076	1.00	2.29	
ATOM	2065	CA	GLU	531	54.246	41.854	77.747	1.00	5.46	
ATOM	2066	CB	GLU	531	54.178	42.919	78.836	1.00	10.50	
ATOM	2067	CG	GLU	531	54.046	42.346	80.257	1.00	12.93	
ATOM	2068	CD	GLU	531	53.771	43.413	81.298	1.00	14.12	
ATOM	2069	OE1	GLU	531	54.085	44.606	81.079	1.00	15.54	
ATOM	2070	OE2	GLU	531	53.227	43.052	82.355	1.00	18.13	
ATOM	2071	C	GLU	531	54.462	42.489	76.382	1.00	6.42	
ATOM	2072	O	GLU	531	53.305	42.685	75.650	1.00	9.10	
ATOM	2073	N	ARG	532	55.659	43.021	76.152	1.00	5.91	
ATOM	2074	CA	ARG	532	56.039	43.529	74.832	1.00	6.83	
ATOM	2075	CB	ARG	532	56.900	44.795	74.890	1.00	6.46	
ATOM	2076	CG	ARG	532	56.141	46.059	75.094	1.00	4.16	
ATOM	2077	CD	ARG	532	55.682	46.070	76.483	1.00	6.94	
ATOM	2078	NE	ARG	532	54.531	46.930	76.696	1.00	14.70	
ATOM	2079	CZ	ARG	532	54.158	47.395	77.890	1.00	17.72	
ATOM	2080	NH1	ARG	532	54.877	47.096	78.975	1.00	19.74	
ATOM	2081	NH2	ARG	532	52.998	48.056	78.017	1.00	18.08	
ATOM	2082	C	ARG	532	56.934	42.364	74.434	1.00	9.68	
ATOM	2083	O	ARG	532	56.904	41.310	75.052	1.00	12.29	
ATOM	2084	N	LEU	533	57.767	42.502	73.436	1.00	10.64	
ATOM	2085	CA	LEU	533	58.606	41.356	73.125	1.00	12.12	
ATOM	2086	CB	LEU	533	58.326	40.790	71.821	1.00	13.13	
ATOM	2087	CG	LEU	533	56.884	40.298	71.741	1.00	10.95	
ATOM	2088	CD1	LEU	533	56.531	39.778	70.348	1.00	11.69	
ATOM	2089	CD2	LEU	533	56.773	39.204	72.754	1.00	12.40	
ATOM	2090	C	LEU	533	60.064	41.733	73.430	1.00	11.85	
ATOM	2091	O	LEU	533	60.897	41.690	72.535	1.00	12.70	
ATOM	2092	N	GLU	534	60.365	42.115	74.666	1.00	12.95	
ATOM	2093	CA	GLU	534	61.722	42.523	75.003	1.00	13.80	
ATOM	2094	CB	GLU	534	61.999	43.882	74.365	1.00	16.94	
ATOM	2095	CG	GLU	534	61.006	44.976	74.791	1.00	23.08	
ATOM	2096	CD	GLU	534	60.768	46.010	73.684	1.00	26.01	
ATOM	2097	OE1	GLU	534	59.849	46.869	73.862	1.00	25.36	
ATOM	2098	OE2	GLU	534	61.461	45.938	72.625	1.00	25.83	

bref21c.pdb Thu Apr 25 12:27:47 1996 28

ATOM	2099	C	GLU	534	61.892	42.579	76.527	1.00	10.95	
ATOM	2100	O	GLU	534	62.651	43.380	77.066	1.00	10.92	
ATOM	2101	N	ASP	535	61.251	41.637	77.194	1.00	9.01	
ATOM	2102	CA	ASP	535	61.247	41.578	78.638	1.00	6.92	
ATOM	2103	CB	ASP	535	60.188	42.544	79.128	1.00	8.31	
ATOM	2104	CG	ASP	535	58.848	42.334	78.430	1.00	8.75	
ATOM	2105	OD1	ASP	535	58.020	41.541	78.913	1.00	11.89	
ATOM	2106	OD2	ASP	535	58.635	42.949	77.372	1.00	15.77	
ATOM	2107	C	ASP	535	60.793	40.201	79.033	1.00	6.27	
ATOM	2108	O	ASP	535	60.062	39.577	78.295	1.00	6.65	
ATOM	2109	N	LEU	536	61.176	39.731	80.204	1.00	5.28	
ATOM	2110	CA	LEU	536	60.717	38.436	80.651	1.00	4.48	
ATOM	2111	CB	LEU	536	61.614	37.315	80.149	1.00	2.00	
ATOM	2112	CG	LEU	536	61.012	35.958	80.495	1.00	2.00	
ATOM	2113	CD1	LEU	536	59.697	35.789	79.782	1.00	2.00	
ATOM	2114	CD2	LEU	536	61.955	34.853	80.152	1.00	2.00	
ATOM	2115	C	LEU	536	60.725	38.468	82.154	1.00	5.42	
ATOM	2116	O	LEU	536	61.701	38.896	82.751	1.00	5.81	
ATOM	2117	N	VAL	537	59.606	38.093	82.767	1.00	6.59	7
ATOM	2118	CA	VAL	537	59.514	38.050	84.219	1.00	4.71	6
ATOM	2119	CB	VAL	537	58.439	39.006	84.761	1.00	3.90	6
ATOM	2120	CG1	VAL	537	58.391	38.900	86.262	1.00	7.66	6
ATOM	2121	CG2	VAL	537	58.754	40.434	84.386	1.00	6.66	6
ATOM	2122	C	VAL	537	59.111	36.652	84.604	1.00	2.70	6
ATOM	2123	O	VAL	537	58.232	36.096	83.977	1.00	5.62	6
ATOM	2124	N	CYS	538	59.812	36.048	85.553	1.00	3.31	7
ATOM	2125	CA	CYS	538	59.452	34.711	86.055	1.00	4.73	6
ATOM	2126	C	CYS	538	59.375	34.771	87.597	1.00	5.86	6
ATOM	2127	O	CYS	538	60.165	35.457	88.257	1.00	6.30	8
ATOM	2128	CB	CYS	538	60.438	33.619	85.600	1.00	2.00	6
ATOM	2129	SG	CYS	538	60.634	33.421	83.795	1.00	3.79	16
ATOM	2130	N	PHE	539	58.426	34.059	88.178	1.00	3.78	7
ATOM	2131	CA	PHE	539	58.267	34.099	89.621	1.00	4.15	6
ATOM	2132	CB	PHE	539	57.295	35.232	89.997	1.00	4.88	6
ATOM	2133	CG	PHE	539	55.852	35.009	89.515	1.00	7.86	6
ATOM	2134	CD1	PHE	539	54.835	34.690	90.420	1.00	5.60	6
ATOM	2135	CD2	PHE	539	55.519	35.104	88.147	1.00	9.65	6
ATOM	2136	CE1	PHE	539	53.540	34.470	89.986	1.00	4.81	6
ATOM	2137	CE2	PHE	539	54.201	34.878	87.706	1.00	7.22	6
ATOM	2138	CZ	PHE	539	53.223	34.562	88.630	1.00	5.52	6
ATOM	2139	C	PHE	539	57.689	32.807	90.123	1.00	3.30	6
ATOM	2140	O	PHE	539	57.397	31.913	89.352	1.00	5.07	8
ATOM	2141	N	TRP	540	57.606	32.696	91.436	1.00	2.62	7
ATOM	2142	CA	TRP	540	56.965	31.575	92.102	1.00	5.41	6
ATOM	2143	CB	TRP	540	57.859	30.331	92.252	1.00	5.13	6
ATOM	2144	CG	TRP	540	58.890	30.380	93.315	1.00	7.06	6
ATOM	2145	CD2	TRP	540	60.250	30.807	93.175	1.00	4.64	6
ATOM	2146	CE2	TRP	540	60.861	30.657	94.430	1.00	5.72	6
ATOM	2147	CE3	TRP	540	61.008	31.299	92.110	1.00	5.86	6
ATOM	2148	CD1	TRP	540	58.738	29.995	94.610	1.00	8.29	6
ATOM	2149	NE1	TRP	540	59.914	30.161	95.286	1.00	8.36	7
ATOM	2150	CZ2	TRP	540	62.208	30.984	94.657	1.00	8.15	6
ATOM	2151	CZ3	TRP	540	62.336	31.623	92.328	1.00	7.58	6
ATOM	2152	CH2	TRP	540	62.927	31.465	93.596	1.00	8.06	6
ATOM	2153	C	TRP	540	56.504	32.189	93.417	1.00	6.24	6
ATOM	2154	O	TRP	540	56.774	33.366	93.668	1.00	7.32	8
ATOM	2155	N	GLU	541	55.698	31.467	94.186	1.00	8.81	7
ATOM	2156	CA	GLU	541	55.187	31.999	95.452	1.00	10.45	6
ATOM	2157	CB	GLU	541	53.768	32.565	95.270	1.00	11.89	6
ATOM	2158	CG	GLU	541	53.592	33.523	94.070	1.00	14.89	6
ATOM	2159	CD	GLU	541	52.202	34.134	93.991	1.00	16.24	6
ATOM	2160	OE1	GLU	541	52.094	35.229	93.415	1.00	17.33	8
ATOM	2161	OE2	GLU	541	51.219	33.550	94.516	1.00	16.64	8
ATOM	2162	C	GLU	541	55.148	30.925	96.507	1.00	10.33	6
ATOM	2163	O	GLU	541	54.744	29.811	96.232	1.00	10.32	8
ATOM	2164	N	GLU	542	55.552	31.242	97.724	1.00	10.91	7
ATOM	2165	CA	GLU	542	55.521	30.222	98.766	1.00	10.78	6
ATOM	2166	CB	GLU	542	56.871	29.482	98.833	1.00	10.24	6
ATOM	2167	CG	GLU	542	58.122	30.359	98.738	1.00	14.40	6
ATOM	2168	CD	GLU	542	59.400	29.571	99.006	1.00	15.97	6
ATOM	2169	OE1	GLU	542	59.711	29.256	100.188	1.00	17.03	8
ATOM	2170	OE2	GLU	542	60.095	29.263	98.026	1.00	17.30	8
ATOM	2171	C	GLU	542	55.082	30.763	100.128	1.00	9.66	6
ATOM	2172	O	GLU	542	54.741	31.947	100.248	1.00	9.88	8
ATOM	2173	N	ALA	543	55.051	29.889	101.135	1.00	8.81	7
ATOM	2174	CA	ALA	543	54.652	30.258	102.493	1.00	7.10	6
ATOM	2175	CB	ALA	543	54.466	29.035	103.325	1.00	4.26	6
ATOM	2176	C	ALA	543	55.716	31.141	103.108	1.00	8.66	6

ATOM	2177	O	ALA	543	56.911	30.849	102.998	1.00	10.83	
ATOM	2178	N	ALA	544	55.286	32.253	103.695	1.00	9.48	
ATOM	2179	CA	ALA	544	56.199	33.185	104.325	1.00	10.43	
ATOM	2180	CB	ALA	544	55.425	34.374	104.890	1.00	11.52	
ATOM	2181	C	ALA	544	56.867	32.397	105.438	1.00	11.84	
ATOM	2182	O	ALA	544	56.169	31.744	106.216	1.00	13.61	
ATOM	2183	N	SER	545	58.204	32.393	105.456	1.00	12.17	
ATOM	2184	CA	SER	545	58.993	31.669	106.453	1.00	13.08	
ATOM	2185	CB	SER	545	59.335	30.251	105.980	1.00	12.98	
ATOM	2186	OG	SER	545	60.291	29.628	106.827	1.00	14.06	
ATOM	2187	C	SER	545	60.245	32.440	106.891	1.00	14.68	
ATOM	2188	O	SER	545	60.865	33.184	106.117	1.00	15.67	
ATOM	2189	N	ALA	546	60.557	32.271	108.174	1.00	17.50	
ATOM	2190	CA	ALA	546	61.639	32.942	108.882	1.00	17.93	
ATOM	2191	CB	ALA	546	61.927	32.215	110.200	1.00	17.78	
ATOM	2192	C	ALA	546	62.928	33.213	108.143	1.00	18.94	
ATOM	2193	O	ALA	546	63.651	32.297	107.751	1.00	19.69	
ATOM	2194	N	GLY	547	63.212	34.495	107.965	1.00	19.34	
ATOM	2195	CA	GLY	547	64.438	34.889	107.300	1.00	20.46	
ATOM	2196	C	GLY	547	64.841	34.140	106.032	1.00	20.86	
ATOM	2197	O	GLY	547	66.045	34.046	105.739	1.00	23.71	
ATOM	2198	N	VAL	548	63.867	33.560	105.322	1.00	18.62	
ATOM	2199	CA	VAL	548	64.111	32.882	104.048	1.00	14.08	
ATOM	2200	CB	VAL	548	63.115	31.749	103.826	1.00	12.71	
ATOM	2201	CG1	VAL	548	63.134	31.309	102.363	1.00	13.62	
ATOM	2202	CG2	VAL	548	63.450	30.579	104.756	1.00	11.28	
ATOM	2203	C	VAL	548	63.874	33.971	102.995	1.00	15.33	
ATOM	2204	O	VAL	548	62.721	34.309	102.714	1.00	16.13	
ATOM	2205	N	GLY	549	64.954	34.612	102.541	1.00	15.42	
ATOM	2206	CA	GLY	549	64.852	35.667	101.551	1.00	12.34	
ATOM	2207	C	GLY	549	65.473	35.180	100.263	1.00	12.73	
ATOM	2208	O	GLY	549	65.765	33.991	100.117	1.00	11.82	
ATOM	2209	N	PRO	550	65.666	36.066	99.283	1.00	12.01	
ATOM	2210	CD	PRO	550	65.213	37.459	99.166	1.00	12.99	
ATOM	2211	CA	PRO	550	66.271	35.639	98.017	1.00	13.59	
ATOM	2212	CB	PRO	550	66.333	36.943	97.199	1.00	9.83	
ATOM	2213	CG	PRO	550	66.201	38.019	98.199	1.00	10.09	
ATOM	2214	C	PRO	550	67.647	34.964	98.157	1.00	13.34	
ATOM	2215	O	PRO	550	67.991	34.066	97.377	1.00	14.83	
ATOM	2216	N	GLY	551	68.384	35.340	99.204	1.00	13.58	
ATOM	2217	CA	GLY	551	69.714	34.797	99.443	1.00	11.00	
ATOM	2218	C	GLY	551	69.776	33.300	99.601	1.00	9.01	
ATOM	2219	O	GLY	551	70.854	32.736	99.588	1.00	11.57	
ATOM	2220	N	ASN	552	68.625	32.655	99.726	1.00	6.84	
ATOM	2221	CA	ASN	552	68.573	31.215	99.888	1.00	6.10	
ATOM	2222	CB	ASN	552	67.510	30.851	100.904	1.00	4.08	
ATOM	2223	CG	ASN	552	67.797	31.449	102.226	1.00	6.03	
ATOM	2224	OD1	ASN	552	68.789	31.112	102.850	1.00	7.24	
ATOM	2225	ND2	ASN	552	66.991	32.411	102.631	1.00	9.39	
ATOM	2226	C	ASN	552	68.287	30.504	98.590	1.00	7.54	
ATOM	2227	O	ASN	552	68.176	29.265	98.580	1.00	7.91	
ATOM	2228	N	TYR	553	68.157	31.278	97.506	1.00	5.28	
ATOM	2229	CA	TYR	553	67.867	30.738	96.186	1.00	4.43	
ATOM	2230	CB	TYR	553	66.432	31.088	95.779	1.00	4.87	
ATOM	2231	CG	TYR	553	65.367	30.341	96.520	1.00	4.46	
ATOM	2232	CD1	TYR	553	64.491	31.001	97.373	1.00	3.71	
ATOM	2233	CE1	TYR	553	63.574	30.290	98.117	1.00	3.40	
ATOM	2234	CD2	TYR	553	65.280	28.953	96.423	1.00	3.40	
ATOM	2235	CE2	TYR	553	64.355	28.243	97.167	1.00	3.44	
ATOM	2236	CZ	TYR	553	63.516	28.914	98.012	1.00	2.00	
ATOM	2237	OH	TYR	553	62.650	28.188	98.778	1.00	3.67	
ATOM	2238	C	TYR	553	68.791	31.287	95.114	1.00	5.08	
ATOM	2239	O	TYR	553	69.432	32.306	95.299	1.00	4.85	
ATOM	2240	N	SER	554	68.845	30.612	93.980	1.00	5.81	
ATOM	2241	CA	SER	554	69.622	31.109	92.865	1.00	6.70	
ATOM	2242	CB	SER	554	70.999	30.456	92.832	1.00	8.42	
ATOM	2243	OG	SER	554	70.954	29.192	92.214	1.00	11.53	
ATOM	2244	C	SER	554	68.800	30.783	91.621	1.00	6.93	
ATOM	2245	O	SER	554	68.289	29.684	91.502	1.00	7.83	
ATOM	2246	N	PHE	555	68.574	31.783	90.773	1.00	6.48	
ATOM	2247	CA	PHE	555	67.811	31.640	89.536	1.00	6.32	
ATOM	2248	CB	PHE	555	66.734	32.730	89.484	1.00	6.75	
ATOM	2249	CG	PHE	555	65.780	32.595	88.335	1.00	5.98	
ATOM	2250	CD1	PHE	555	64.622	32.509	88.567	1.00	3.96	
ATOM	2251	CD2	PHE	555	66.242	32.554	87.319	1.00	4.43	
ATOM	2252	CE1	PHE	555	63.541	32.382	87.507	1.00	6.29	
ATOM	2253	CE2	PHE	555	65.379	32.427	85.963	1.00	3.92	
ATOM	2254	CZ	PHE	555	64.030	32.339	86.196	1.00	5.62	

bref21c.pdb Thu Apr 25 12:27:47 1996 30

```
ATOM   2255  C   PHE   555      68.779  31.759  68.337  1.00  6.86
ATOM   2256  O   PHE   555      69.184  32.858  67.965  1.00  8.43
ATOM   2257  N   SER   556      69.095  30.616  67.740  1.00  7.22
ATOM   2258  CA  SER   556      70.019  30.503  66.619  1.00  6.83
ATOM   2259  CB  SER   556      70.969  29.315  66.879  1.00  4.30
ATOM   2260  OG  SER   556      71.923  29.587  67.891  1.00  8.78
ATOM   2261  C   SER   556      69.336  30.298  65.257  1.00  5.62
ATOM   2262  O   SER   556      68.535  29.389  65.117  1.00  8.35
ATOM   2263  N   TYR   557      69.682  31.102  64.255  1.00  3.08
ATOM   2264  CA  TYR   557      69.123  30.943  62.924  1.00  3.30
ATOM   2265  CB  TYR   557      68.198  32.089  62.569  1.00  2.00
ATOM   2266  CG  TYR   557      68.832  33.434  62.422  1.00  2.00
ATOM   2267  CD1 TYR   557      69.405  33.825  81.218  1.00  2.00
ATOM   2268  CE1 TYR   557      69.851  35.126  61.023  1.00  2.56
ATOM   2269  CD2 TYR   557      68.737  34.368  63.434  1.00  2.00
ATOM   2270  CE2 TYR   557      69.184  35.667  63.260  1.00  2.00
ATOM   2271  CZ  TYR   557      69.734  36.047  62.051  1.00  3.10
ATOM   2272  OH  TYR   557      70.124  37.356  61.865  1.00  3.23
ATOM   2273  C   TYR   557      70.191  30.834  61.870  1.00  3.33
ATOM   2274  O   TYR   557      71.316  31.196  62.090  1.00  4.25
ATOM   2275  N   GLN   558      69.839  30.360  60.695  1.00  3.52
ATOM   2276  CA  GLN   558      70.831  30.227  59.648  1.00  3.20
ATOM   2277  CB  GLN   558      71.603  28.925  59.828  1.00  3.66
ATOM   2278  CG  GLN   558      72.506  28.598  58.648  1.00  6.55
ATOM   2279  CD  GLN   558      73.171  27.282  58.788  1.00  5.14
ATOM   2280  OE1 GLN   558      72.552  26.320  59.183  1.00  6.68
ATOM   2281  NE2 GLN   558      74.447  27.229  58.477  1.00  7.23
ATOM   2282  C   GLN   558      70.204  30.208  58.279  1.00  3.24
ATOM   2283  O   GLN   558      69.420  29.309  57.977  1.00  2.96
ATOM   2284  N   LEU   559      70.518  31.189  57.445  1.00  2.00
ATOM   2285  CA  LEU   559      69.945  31.139  56.120  1.00  2.89
ATOM   2286  CB  LEU   559      70.036  32.487  55.399  1.00  2.00
ATOM   2287  CG  LEU   559      68.975  33.527  55.792  1.00  2.00
ATOM   2288  CD1 LEU   559      69.103  34.810  55.005  1.00  2.00
ATOM   2289  CD2 LEU   559      67.612  32.955  55.564  1.00  2.00
ATOM   2290  C   LEU   559      70.764  30.060  55.447  1.00  5.30
ATOM   2291  O   LEU   559      71.951  29.947  55.728  1.00  4.67
ATOM   2292  N   GLU   560      70.091  29.169  54.718  1.00  6.97
ATOM   2293  CA  GLU   560      70.737  28.064  53.997  1.00 11.03
ATOM   2294  CB  GLU   560      69.787  27.517  52.938  1.00 14.40
ATOM   2295  CG  GLU   560      70.290  26.305  52.163  1.00 19.08
ATOM   2296  CD  GLU   560      69.701  26.207  50.738  1.00 20.20
ATOM   2297  OE1 GLU   560      69.790  27.202  49.983  1.00 25.39
ATOM   2298  OE2 GLU   560      69.200  25.130  50.346  1.00 21.83
ATOM   2299  C   GLU   560      71.995  28.572  53.310  1.00 11.71
ATOM   2300  O   GLU   560      71.919  29.491  52.505  1.00 10.88
ATOM   2301  N   ASP   561      73.140  27.970  53.648  1.00 12.36
ATOM   2302  CA  ASP   561      74.460  28.346  53.118  1.00 13.20
ATOM   2303  CB  ASP   561      74.478  28.398  51.589  1.00 11.29
ATOM   2304  CG  ASP   561      74.440  27.038  50.968  1.00 13.29
ATOM   2305  OD1 ASP   561      74.530  26.039  51.725  1.00 14.53
ATOM   2306  OD2 ASP   561      74.296  26.963  49.729  1.00 11.84
ATOM   2307  C   ASP   561      74.995  29.667  53.661  1.00 17.27
ATOM   2308  O   ASP   561      75.663  30.426  52.931  1.00 21.27
ATOM   2309  N   GLU   562      74.714  29.972  54.926  1.00 17.40
ATOM   2310  CA  GLU   562      75.220  31.218  55.504  1.00 16.45
ATOM   2311  CB  GLU   562      74.092  32.235  55.652  1.00 20.22
ATOM   2312  CG  GLU   562      73.224  32.450  54.408  1.00 23.17
ATOM   2313  CD  GLU   562      73.909  33.234  53.289  1.00 23.82
ATOM   2314  OE1 GLU   562      74.330  34.407  53.511  1.00 22.18
ATOM   2315  OE2 GLU   562      73.981  32.670  52.169  1.00 27.47
ATOM   2316  C   GLU   562      75.764  30.847  56.871  1.00 14.28
ATOM   2317  O   GLU   562      75.431  29.759  57.373  1.00 16.94
ATOM   2318  N   PRO   563      76.662  31.681  57.465  1.00 11.29
ATOM   2319  CD  PRO   563      77.200  33.009  57.064  1.00  5.24
ATOM   2320  CA  PRO   563      77.156  31.287  58.794  1.00 11.69
ATOM   2321  CB  PRO   563      78.186  32.376  59.111  1.00  7.10
ATOM   2322  CG  PRO   563      77.655  33.548  58.404  1.00  6.79
ATOM   2323  C   PRO   563      75.965  31.277  59.788  1.00 10.73
ATOM   2324  O   PRO   563      74.981  32.001  59.558  1.00 11.36
ATOM   2325  N   TRP   564      75.995  30.362  80.772  1.00  8.20
ATOM   2326  CA  TRP   564      76.945  30.255  81.806  1.00  5.30
ATOM   2327  CB  TRP   564      75.304  29.199  82.845  1.00  2.55
ATOM   2328  CG  TRP   564      74.650  27.886  82.700  1.00  5.38
ATOM   2329  CD2 TRP   564      73.276  27.585  82.941  1.00  6.62
ATOM   2330  CE2 TRP   564      73.116  26.188  82.761  1.00  6.86
ATOM   2331  CE3 TRP   564      72.158  28.357  83.296  1.00  8.59
ATOM   2332  CD1 TRP   564      75.250  26.709  82.387  1.00  6.26
```

```
ATOM   2333  NE1 TRP   564      74.338  25.675  82.422  1.00  5.36
ATOM   2334  CZ2 TRP   564      71.880  25.546  82.929  1.00  6.49
ATOM   2335  CZ3 TRP   564      70.928  27.723  83.461  1.00  6.79
ATOM   2336  CH2 TRP   564      70.801  26.328  83.279  1.00  8.18
ATOM   2337  C   TRP   564      74.880  31.597  82.525  1.00  5.66
ATOM   2338  O   TRP   564      75.908  32.259  82.740  1.00  9.32
ATOM   2339  N   LYS   565      73.690  31.997  82.927  1.00  3.69
ATOM   2340  CA  LYS   565      73.542  33.256  83.612  1.00  2.00
ATOM   2341  CB  LYS   565      73.099  34.332  82.625  1.00  2.00
ATOM   2342  CG  LYS   565      74.242  34.886  81.791  1.00  2.00
ATOM   2343  CD  LYS   565      73.827  35.197  80.371  1.00  3.81
ATOM   2344  CE  LYS   565      74.814  36.116  79.711  1.00  3.15
ATOM   2345  NZ  LYS   565      74.856  37.374  80.497  1.00  6.31
ATOM   2346  C   LYS   565      72.669  33.171  84.878  1.00  3.24
ATOM   2347  O   LYS   565      71.856  32.270  85.043  1.00  2.53
ATOM   2348  N   LEU   566      72.863  34.113  85.783  1.00  3.46
ATOM   2349  CA  LEU   566      72.160  34.100  87.042  1.00  6.16
ATOM   2350  CB  LEU   566      73.187  33.857  88.143  1.00  7.13
ATOM   2351  CG  LEU   566      72.902  33.890  89.641  1.00 11.04
ATOM   2352  CD1 LEU   566      74.121  33.292  90.343  1.00 13.73
ATOM   2353  CD2 LEU   566      72.660  35.299  90.155  1.00 11.29
ATOM   2354  C   LEU   566      71.505  35.418  87.265  1.00  6.69
ATOM   2355  O   LEU   566      72.175  36.430  87.315  1.00  6.80
ATOM   2356  N   CYS   567      70.199  35.446  87.406  1.00  7.27
ATOM   2357  CA  CYS   567      69.636  36.738  87.658  1.00 10.28
ATOM   2358  C   CYS   567      69.245  37.013  89.124  1.00 13.20
ATOM   2359  O   CYS   567      69.271  36.118  89.983  1.00 13.64
ATOM   2360  CB  CYS   567      68.506  37.017  86.707  1.00 12.97
ATOM   2361  SG  CYS   567      67.190  35.797  86.808  1.00 17.32
ATOM   2362  N   ARG   568      69.009  38.293  89.405  1.00 15.13
ATOM   2363  CA  ARG   568      68.626  38.777  90.727  1.00 14.78
ATOM   2364  CB  ARG   568      68.781  40.310  90.798  1.00 17.37
ATOM   2365  CG  ARG   568      70.037  40.829  91.510  1.00 20.45
ATOM   2366  CD  ARG   568      71.329  40.711  90.681  1.00 20.67
ATOM   2367  NE  ARG   568      72.045  41.996  90.624  1.00 22.26
ATOM   2368  CZ  ARG   568      72.587  42.642  91.671  1.00 22.85
ATOM   2369  NH1 ARG   568      72.531  42.151  92.918  1.00 20.25
ATOM   2370  NH2 ARG   568      73.191  43.816  91.465  1.00 24.23
ATOM   2371  C   ARG   568      67.185  38.399  91.086  1.00 14.39
ATOM   2372  O   ARG   568      66.247  38.690  90.329  1.00 15.75
ATOM   2373  N   LEU   569      67.046  37.752  92.248  1.00 11.39
ATOM   2374  CA  LEU   569      65.782  37.304  92.807  1.00  6.32
ATOM   2375  CB  LEU   569      66.005  36.101  93.715  1.00  2.00
ATOM   2376  CG  LEU   569      65.069  34.917  93.607  1.00  3.41
ATOM   2377  CD1 LEU   569      64.374  34.905  92.287  1.00  3.80
ATOM   2378  CD2 LEU   569      65.852  33.675  93.759  1.00  2.00
ATOM   2379  C   LEU   569      65.318  36.461  93.637  1.00  7.64
ATOM   2380  O   LEU   569      66.121  29.228  94.131  1.00  6.24
ATOM   2381  N   HIS   570      64.015  38.644  93.719  1.00  9.65
ATOM   2382  CA  HIS   570      63.454  39.712  94.531  1.00 10.84
ATOM   2383  CB  HIS   570      62.841  40.811  93.655  1.00 11.04
ATOM   2384  CG  HIS   570      63.820  41.547  92.802  1.00 10.81
ATOM   2385  CD2 HIS   570      64.739  42.492  93.108  1.00 13.10
ATOM   2386  ND1 HIS   570      63.845  41.421  91.431  1.00 14.00
ATOM   2387  CE1 HIS   570      64.728  42.263  90.925  1.00 14.17
ATOM   2388  NE2 HIS   570      65.285  42.925  91.924  1.00 12.65
ATOM   2389  C   HIS   570      62.359  39.076  95.393  1.00  9.92
ATOM   2390  O   HIS   570      62.098  37.884  95.284  1.00 14.44
ATOM   2391  N   GLN   571      61.725  39.869  96.246  1.00  9.24
ATOM   2392  CA  GLN   571      60.655  39.368  97.063  1.00  6.37
ATOM   2393  CB  GLN   571      61.187  38.806  98.371  1.00 11.43
ATOM   2394  CG  GLN   571      60.150  38.017  99.168  1.00 13.27
ATOM   2395  CD  GLN   571      60.187  38.342 100.666  1.00 21.53
ATOM   2396  OE1 GLN   571      61.169  38.037 101.358  1.00 22.69
ATOM   2397  NE2 GLN   571      59.116  38.962 101.170  1.00 22.76
ATOM   2398  C   GLN   571      59.712  40.504  97.308  1.00  3.52
ATOM   2399  O   GLN   571      60.098  41.656  97.285  1.00  2.00
ATOM   2400  N   ALA   572      58.445  40.152  97.419  1.00  4.26
ATOM   2401  CA  ALA   572      57.348  41.081  97.658  1.00  5.12
ATOM   2402  CB  ALA   572      56.920  41.774  96.356  1.00  2.27
ATOM   2403  C   ALA   572      56.217  40.214  98.195  1.00  4.95
ATOM   2404  O   ALA   572      56.260  38.979  98.057  1.00  6.25
ATOM   2405  N   PRO   573      55.213  40.823  98.864  1.00  8.54
ATOM   2406  CD  PRO   573      55.084  42.102  99.602  1.00  6.45
ATOM   2407  CA  PRO   573      54.205  39.868  99.323  1.00  8.35
ATOM   2408  CB  PRO   573      53.769  40.437 100.696  1.00  9.62
ATOM   2409  CG  PRO   573      54.785  41.599 100.984  1.00  7.39
ATOM   2410  C   PRO   573      53.044  39.734  98.377  1.00  7.83
```

bref21c.pdb Thu Apr 25 12:27:47 1996 32

ATOM	2411	O	PRO	573	52.768	40.608	97.552	1.00	7.72	5
ATOM	2412	N	THR	574	52.428	38.574	98.476	1.00	8.95	5
ATOM	2413	CA	THR	574	51.255	38.232	97.727	1.00	10.96	6
ATOM	2414	CB	THR	574	51.075	36.738	97.733	1.00	10.37	6
ATOM	2415	OG1	THR	574	52.135	36.153	96.980	1.00	14.24	8
ATOM	2416	CG2	THR	574	49.712	36.324	97.155	1.00	13.72	6
ATOM	2417	C	THR	574	50.119	38.852	98.515	1.00	12.85	6
ATOM	2418	O	THR	574	50.163	38.874	99.752	1.00	14.59	8
ATOM	2419	N	ALA	575	49.087	39.324	97.812	1.00	14.88	7
ATOM	2420	CA	ALA	575	47.934	39.946	98.467	1.00	14.50	6
ATOM	2421	CB	ALA	575	46.922	40.433	97.439	1.00	14.72	6
ATOM	2422	C	ALA	575	47.282	38.960	99.443	1.00	14.38	6
ATOM	2423	O	ALA	575	46.480	39.355	100.286	1.00	15.91	8
ATOM	2424	N	ARG	576	47.682	37.695	99.344	1.00	12.79	7
ATOM	2425	CA	ARG	576	47.178	36.637	100.189	1.00	11.82	6
ATOM	2426	CB	ARG	576	46.877	35.414	99.328	1.00	15.95	6
ATOM	2427	CG	ARG	576	45.534	35.451	98.604	1.00	20.92	6
ATOM	2428	CD	ARG	576	45.633	34.621	97.302	1.00	24.61	6
ATOM	2429	NE	ARG	576	44.350	34.081	96.848	1.00	27.37	7
ATOM	2430	CZ	ARG	576	44.171	33.438	95.687	1.00	28.99	6
ATOM	2431	NH1	ARG	576	45.188	33.261	94.833	1.00	29.46	7
ATOM	2432	NH2	ARG	576	42.979	32.928	95.391	1.00	27.90	7
ATOM	2433	C	ARG	576	48.090	36.216	101.351	1.00	9.90	6
ATOM	2434	O	ARG	576	47.843	35.177	101.972	1.00	8.14	8
ATOM	2435	N	GLY	577	49.167	36.963	101.606	1.00	10.36	7
ATOM	2436	CA	GLY	577	50.066	36.615	102.705	1.00	9.58	6
ATOM	2437	C	GLY	577	51.201	35.638	102.425	1.00	11.02	6
ATOM	2438	O	GLY	577	51.959	35.280	103.356	1.00	10.42	8
ATOM	2439	N	ALA	578	51.262	35.140	101.193	1.00	11.51	7
ATOM	2440	CA	ALA	578	52.332	34.245	100.720	1.00	10.32	6
ATOM	2441	CB	ALA	578	51.842	33.360	99.617	1.00	6.95	6
ATOM	2442	C	ALA	578	53.443	35.158	100.212	1.00	10.21	6
ATOM	2443	O	ALA	578	53.278	36.384	100.138	1.00	9.88	8
ATOM	2444	N	VAL	579	54.597	34.593	99.905	1.00	9.95	7
ATOM	2445	CA	VAL	579	55.673	35.431	99.406	1.00	10.55	6
ATOM	2446	CB	VAL	579	56.957	35.294	100.247	1.00	9.32	6
ATOM	2447	CG1	VAL	579	56.734	35.863	101.618	1.00	8.45	6
ATOM	2448	CG2	VAL	579	57.363	33.860	100.350	1.00	11.44	6
ATOM	2449	C	VAL	579	55.923	35.128	97.939	1.00	9.09	6
ATOM	2450	O	VAL	579	55.599	34.044	97.452	1.00	8.40	8
ATOM	2451	N	ARG	580	56.460	36.104	97.229	1.00	7.06	7
ATOM	2452	CA	ARG	580	56.721	35.917	95.816	1.00	7.86	6
ATOM	2453	CB	ARG	580	55.769	36.792	94.991	1.00	8.84	6
ATOM	2454	CG	ARG	580	55.926	36.721	93.503	1.00	7.88	6
ATOM	2455	CD	ARG	580	55.080	37.813	92.844	1.00	8.78	6
ATOM	2456	NE	ARG	580	53.652	37.517	92.913	1.00	6.85	7
ATOM	2457	CZ	ARG	580	52.719	38.362	93.341	1.00	5.69	6
ATOM	2458	NH1	ARG	580	53.050	39.581	93.731	1.00	5.12	7
ATOM	2459	NH2	ARG	580	51.470	37.952	93.466	1.00	2.00	7
ATOM	2460	C	ARG	580	58.159	36.282	95.523	1.00	7.72	6
ATOM	2461	O	ARG	580	58.664	37.321	95.954	1.00	7.66	8
ATOM	2462	N	PHE	581	58.827	35.387	94.827	1.00	6.07	7
ATOM	2463	CA	PHE	581	60.200	35.596	94.458	1.00	5.52	6
ATOM	2464	CB	PHE	581	60.982	34.355	94.803	1.00	4.84	6
ATOM	2465	CG	PHE	581	61.274	34.214	96.250	1.00	4.90	6
ATOM	2466	CD1	PHE	581	60.510	33.372	97.045	1.00	3.60	6
ATOM	2467	CD2	PHE	581	62.371	34.883	96.822	1.00	5.69	6
ATOM	2468	CE1	PHE	581	60.835	33.191	98.390	1.00	4.44	6
ATOM	2469	CE2	PHE	581	62.694	34.700	98.165	1.00	5.88	6
ATOM	2470	CZ	PHE	581	61.926	33.854	98.944	1.00	3.43	6
ATOM	2471	C	PHE	581	60.287	35.939	92.961	1.00	5.46	6
ATOM	2472	O	PHE	581	59.686	35.101	92.194	1.00	6.33	8
ATOM	2473	N	TRP	582	61.037	36.844	92.525	1.00	6.16	7
ATOM	2474	CA	TRP	582	61.129	37.054	91.090	1.00	7.26	6
ATOM	2475	CB	TRP	582	59.861	37.778	90.589	1.00	9.34	6
ATOM	2476	CG	TRP	582	59.462	38.933	91.423	1.00	10.74	6
ATOM	2477	CD2	TRP	582	59.916	40.268	91.280	1.00	11.49	6
ATOM	2478	CE2	TRP	582	59.366	41.017	92.359	1.00	11.22	6
ATOM	2479	CE3	TRP	582	60.744	40.906	90.356	1.00	11.65	6
ATOM	2480	CD1	TRP	582	58.663	38.915	92.530	1.00	14.19	6
ATOM	2481	NE1	TRP	582	58.604	40.165	93.105	1.00	12.18	7
ATOM	2482	CZ2	TRP	582	59.618	42.365	92.538	1.00	12.31	6
ATOM	2483	CZ3	TRP	582	61.001	42.247	90.524	1.00	15.91	6
ATOM	2484	CH2	TRP	582	60.436	42.973	91.617	1.00	16.33	6
ATOM	2485	C	TRP	582	62.409	37.622	90.429	1.00	7.94	6
ATOM	2486	O	TRP	582	63.219	38.299	91.041	1.00	6.37	8
ATOM	2487	N	CYS	583	62.556	37.312	89.150	1.00	7.90	7
ATOM	2488	CA	CYS	583	63.656	37.766	88.334	1.00	9.15	6

ATOM	2489	C	CYS	583	63.154	38.449	87.073	1.00	8.52	3
ATOM	2490	O	CYS	583	62.143	38.055	86.520	1.00	8.13	3
ATOM	2491	CB	CYS	583	64.507	36.591	87.876	1.00	11.02	3
ATOM	2492	SG	CYS	583	65.603	36.996	86.470	1.00	12.88	1
ATOM	2493	N	SER	584	63.895	39.453	86.606	1.00	11.08	7
ATOM	2494	CA	SER	584	63.556	40.150	85.375	1.00	11.13	4
ATOM	2495	CB	SER	584	63.210	41.612	85.649	1.00	14.00	4
ATOM	2496	OG	SER	584	62.296	42.141	84.680	1.00	22.72	5
ATOM	2497	C	SER	584	64.819	40.052	84.531	1.00	11.03	4
ATOM	2498	O	SER	584	65.874	40.485	84.990	1.00	14.12	5
ATOM	2499	N	LEU	585	64.743	39.357	83.390	1.00	8.82	7
ATOM	2500	CA	LEU	585	65.889	39.214	82.500	1.00	7.31	4
ATOM	2501	CB	LEU	585	65.638	38.192	81.374	1.00	5.24	6
ATOM	2502	CG	LEU	585	65.265	36.731	81.541	1.00	2.00	6
ATOM	2503	CD1	LEU	585	65.929	35.888	80.486	1.00	2.00	6
ATOM	2504	CD2	LEU	585	65.633	36.271	82.912	1.00	5.67	6
ATOM	2505	C	LEU	585	66.134	40.562	81.832	1.00	8.79	6
ATOM	2506	O	LEU	585	65.188	41.282	81.508	1.00	7.56	8
ATOM	2507	N	PRO	586	67.410	40.929	81.637	1.00	10.50	7
ATOM	2508	CD	PRO	586	68.622	40.279	82.160	1.00	12.29	6
ATOM	2509	CA	PRO	586	67.746	42.202	80.993	1.00	11.85	6
ATOM	2510	CB	PRO	586	69.257	42.304	81.191	1.00	11.45	6
ATOM	2511	CG	PRO	586	69.505	41.470	82.416	1.00	13.83	6
ATOM	2512	C	PRO	586	67.416	42.019	79.520	1.00	14.14	6
ATOM	2513	O	PRO	586	67.834	41.019	78.912	1.00	14.17	8
ATOM	2514	N	THR	587	66.691	42.985	78.957	1.00	13.17	7
ATOM	2515	CA	THR	587	66.261	42.949	77.569	1.00	12.49	6
ATOM	2516	CB	THR	587	66.168	44.355	76.969	1.00	15.17	6
ATOM	2517	OG1	THR	587	65.927	45.330	78.002	1.00	18.67	8
ATOM	2518	CG2	THR	587	65.049	44.408	75.929	1.00	17.05	6
ATOM	2519	C	THR	587	67.182	42.186	76.657	1.00	12.00	6
ATOM	2520	O	THR	587	66.739	41.308	75.948	1.00	11.83	8
ATOM	2521	N	ALA	588	68.472	42.530	76.700	1.00	11.51	7
ATOM	2522	CA	ALA	588	69.513	41.927	75.849	1.00	7.86	6
ATOM	2523	CB	ALA	588	70.896	42.342	76.320	1.00	8.95	6
ATOM	2524	C	ALA	588	69.435	40.425	75.700	1.00	7.36	5
ATOM	2525	O	ALA	588	69.825	39.894	74.681	1.00	8.37	8
ATOM	2526	N	ASP	589	68.877	39.747	76.693	1.00	7.82	7
ATOM	2527	CA	ASP	589	68.745	38.300	76.651	1.00	7.85	5
ATOM	2528	CB	ASP	589	69.173	37.684	77.976	1.00	5.24	6
ATOM	2529	CG	ASP	589	70.673	37.683	78.168	1.00	5.26	6
ATOM	2530	OD1	ASP	589	71.088	38.045	79.298	1.00	6.38	8
ATOM	2531	OD2	ASP	589	71.422	37.299	77.230	1.00	2.00	8
ATOM	2532	C	ASP	589	67.341	37.845	76.376	1.00	7.96	8
ATOM	2533	O	ASP	589	67.080	36.659	76.383	1.00	7.86	5
ATOM	2534	N	THR	590	66.435	38.780	76.133	1.00	8.88	7
ATOM	2535	CA	THR	590	65.040	38.451	75.899	1.00	10.02	8
ATOM	2536	CB	THR	590	64.118	39.571	76.426	1.00	8.46	8
ATOM	2537	OG1	THR	590	64.496	40.806	75.845	1.00	7.66	8
ATOM	2538	CG2	THR	590	64.269	39.728	77.928	1.00	10.59	3
ATOM	2539	C	THR	590	64.696	38.106	74.465	1.00	10.88	5
ATOM	2540	O	THR	590	63.610	38.414	74.007	1.00	15.28	8
ATOM	2541	N	SER	591	65.592	37.405	73.783	1.00	11.68	7
ATOM	2542	CA	SER	591	65.372	37.022	72.391	1.00	11.91	6
ATOM	2543	CB	SER	591	66.692	36.681	71.696	1.00	13.98	4
ATOM	2544	OG	SER	591	67.046	37.715	70.790	1.00	16.79	8
ATOM	2545	C	SER	591	64.405	35.867	72.177	1.00	11.64	8
ATOM	2546	O	SER	591	64.456	34.847	72.882	1.00	12.56	8
ATOM	2547	N	SER	592	63.585	35.999	71.135	1.00	9.34	7
ATOM	2548	CA	SER	592	62.607	34.988	70.803	1.00	5.84	4
ATOM	2549	CB	SER	592	61.395	35.633	70.119	1.00	6.26	4
ATOM	2550	OG	SER	592	60.795	36.638	70.916	1.00	5.45	8
ATOM	2551	C	SER	592	63.216	33.945	69.869	1.00	5.35	4
ATOM	2552	O	SER	592	64.386	33.974	69.563	1.00	4.72	4
ATOM	2553	N	PHE	593	62.388	32.980	69.537	1.00	5.79	7
ATOM	2554	CA	PHE	593	62.715	31.900	68.620	1.00	8.33	4
ATOM	2555	CB	PHE	593	62.866	32.474	67.189	1.00	7.57	4
ATOM	2556	CG	PHE	593	61.744	33.458	66.791	1.00	6.76	4
ATOM	2557	CD1	PHE	593	62.041	34.679	66.197	1.00	9.27	4
ATOM	2558	CD2	PHE	593	60.399	33.162	67.043	1.00	5.23	4
ATOM	2559	CE1	PHE	593	61.020	35.584	65.866	1.00	9.60	4
ATOM	2560	CE2	PHE	593	59.380	34.054	66.719	1.00	9.02	4
ATOM	2561	CZ	PHE	593	59.686	35.262	66.121	1.00	7.44	4
ATOM	2562	C	PHE	593	63.848	30.947	69.000	1.00	9.84	4
ATOM	2563	O	PHE	593	64.302	30.177	68.151	1.00	11.09	4
ATOM	2564	N	VAL	594	64.223	30.958	70.291	1.00	9.82	7
ATOM	2565	CA	VAL	594	65.284	30.113	70.951	1.00	8.29	4
ATOM	2566	CB	VAL	594	66.588	30.909	71.155	1.00	9.17	4

bref21c.pdb Thu Apr 25 12:27:47 1996 34

ATOM	2567	CG1	VAL	594	67.086	31.490	69.894	1.00	11.27	
ATOM	2568	CG2	VAL	594	66.359	32.005	72.175	1.00	8.98	
ATOM	2569	C	VAL	594	64.874	29.552	72.261	1.00	6.86	
ATOM	2570	O	VAL	594	64.201	30.239	73.037	1.00	9.44	
ATOM	2571	N	PRO	595	65.287	28.308	72.572	1.00	4.06	
ATOM	2572	CD	PRO	595	65.910	27.414	71.592	1.00	4.50	
ATOM	2573	CA	PRO	595	65.040	27.558	73.802	1.00	4.33	
ATOM	2574	CB	PRO	595	65.623	26.185	73.468	1.00	4.07	
ATOM	2575	CG	PRO	595	65.442	26.084	72.064	1.00	2.00	
ATOM	2576	C	PRO	595	65.728	26.142	75.048	1.00	3.58	
ATOM	2577	O	PRO	595	66.955	28.077	75.180	1.00	3.03	
ATOM	2578	N	LEU	596	64.923	28.692	75.955	1.00	3.21	
ATOM	2579	CA	LEU	596	65.420	29.282	77.199	1.00	4.16	
ATOM	2580	CB	LEU	596	64.670	30.596	77.561	1.00	3.29	
ATOM	2581	CG	LEU	596	65.384	31.870	78.068	1.00	2.00	
ATOM	2582	CD1	LEU	596	64.500	32.639	79.002	1.00	3.47	
ATOM	2583	CD2	LEU	596	66.646	31.534	78.783	1.00	2.16	
ATOM	2584	C	LEU	596	65.252	28.293	78.347	1.00	4.67	
ATOM	2585	O	LEU	596	64.121	27.938	78.721	1.00	2.52	
ATOM	2586	N	GLU	597	66.384	27.861	78.900	1.00	4.53	
ATOM	2587	CA	GLU	597	66.406	26.943	80.031	1.00	3.76	
ATOM	2588	CB	GLU	597	67.566	25.980	79.909	1.00	2.00	
ATOM	2589	CG	GLU	597	67.699	25.125	81.113	1.00	2.00	
ATOM	2590	CD	GLU	597	68.548	23.955	80.855	1.00	5.62	
ATOM	2591	OE1	GLU	597	69.206	23.971	79.805	1.00	10.01	
ATOM	2592	OE2	GLU	597	68.562	23.014	81.675	1.00	6.65	
ATOM	2593	C	GLU	597	66.483	27.704	81.367	1.00	2.57	
ATOM	2594	O	GLU	597	67.322	26.596	81.536	1.00	3.19	
ATOM	2595	N	LEU	598	65.590	27.358	82.296	1.00	3.03	
ATOM	2596	CA	LEU	598	65.519	28.001	83.600	1.00	2.16	
ATOM	2597	CB	LEU	598	64.159	28.670	83.777	1.00	2.00	
ATOM	2598	CG	LEU	598	63.756	29.657	82.681	1.00	2.00	
ATOM	2599	CD1	LEU	598	62.279	29.702	82.601	1.00	2.00	
ATOM	2600	CD2	LEU	598	64.368	31.027	82.888	1.00	2.00	
ATOM	2601	C	LEU	598	65.761	26.988	84.700	1.00	2.92	
ATOM	2602	O	LEU	598	65.337	25.833	84.605	1.00	2.64	
ATOM	2603	N	ARG	599	66.462	27.428	85.736	1.00	2.34	
ATOM	2604	CA	ARG	599	66.804	26.580	86.862	1.00	3.62	
ATOM	2605	CB	ARG	599	68.254	26.115	86.710	1.00	6.78	
ATOM	2606	CG	ARG	599	68.479	24.611	86.512	1.00	10.90	
ATOM	2607	CD	ARG	599	69.385	24.359	85.308	1.00	14.84	
ATOM	2608	NE	ARG	599	69.658	22.945	85.047	1.00	17.19	
ATOM	2609	CZ	ARG	599	70.176	22.100	85.942	1.00	17.80	
ATOM	2610	NH1	ARG	599	70.472	22.515	87.182	1.00	17.23	
ATOM	2611	NH2	ARG	599	70.452	20.845	85.580	1.00	15.70	
ATOM	2612	C	ARG	599	66.717	27.367	88.150	1.00	3.41	
ATOM	2613	O	ARG	599	67.394	28.364	88.259	1.00	4.23	
ATOM	2614	N	VAL	600	65.843	26.979	89.081	1.00	2.87	
ATOM	2615	CA	VAL	600	65.756	27.644	90.387	1.00	2.87	
ATOM	2616	CB	VAL	600	64.322	28.001	90.825	1.00	2.92	
ATOM	2617	CG1	VAL	600	64.336	28.512	92.248	1.00	2.20	
ATOM	2618	CG2	VAL	600	63.737	29.035	89.917	1.00	2.00	
ATOM	2619	C	VAL	600	66.272	26.622	91.371	1.00	3.23	
ATOM	2620	O	VAL	600	65.744	25.525	91.426	1.00	4.11	
ATOM	2621	N	THR	601	67.309	26.963	92.124	1.00	5.21	
ATOM	2622	CA	THR	601	67.881	25.043	93.098	1.00	6.74	
ATOM	2623	CB	THR	601	69.296	25.601	92.688	1.00	8.50	
ATOM	2624	OG1	THR	601	69.228	24.939	91.430	1.00	12.77	
ATOM	2625	CG2	THR	601	69.890	24.631	93.684	1.00	8.70	
ATOM	2626	C	THR	601	67.995	26.634	94.481	1.00	8.78	
ATOM	2627	O	THR	601	68.267	27.822	94.637	1.00	11.77	
ATOM	2628	N	ALA	602	67.788	25.792	95.484	1.00	9.87	
ATOM	2629	CA	ALA	602	67.915	26.196	96.877	1.00	9.62	
ATOM	2630	CB	ALA	602	67.254	25.191	97.745	1.00	9.55	
ATOM	2631	C	ALA	602	69.404	26.180	97.153	1.00	10.39	
ATOM	2632	O	ALA	602	70.107	25.324	96.613	1.00	11.86	
ATOM	2633	N	ALA	603	69.872	27.069	98.036	1.00	9.75	
ATOM	2634	CA	ALA	603	71.292	27.162	98.415	1.00	7.23	
ATOM	2635	CB	ALA	603	71.517	28.370	99.300	1.00	6.77	
ATOM	2636	C	ALA	603	71.871	25.882	99.070	1.00	6.03	
ATOM	2637	O	ALA	603	73.066	25.785	99.320	1.00	4.90	
ATOM	2638	N	SER	604	71.026	24.892	99.324	1.00	5.87	
ATOM	2639	CA	SER	604	71.497	23.639	99.897	1.00	7.44	
ATOM	2640	CB	SER	604	70.409	22.980	100.740	1.00	6.33	
ATOM	2641	OG	SER	604	69.702	22.024	99.997	1.00	5.42	
ATOM	2642	C	SER	604	71.914	22.689	98.777	1.00	9.15	
ATOM	2643	O	SER	604	72.462	21.617	99.042	1.00	11.68	
ATOM	2644	N	GLY	605	71.604	23.070	97.535	1.00	7.29	

ATOM	2645	CA	GLY	605	71.944	22.262	96.378	1.00	8.17	
ATOM	2646	C	GLY	605	70.709	21.620	95.785	1.00	7.43	
ATOM	2647	O	GLY	605	70.711	21.198	94.631	1.00	8.81	
ATOM	2648	N	ALA	606	69.639	21.606	96.573	1.00	7.11	
ATOM	2649	CA	ALA	606	68.376	21.001	96.194	1.00	6.20	
ATOM	2650	CB	ALA	606	67.492	20.885	97.387	1.00	2.64	
ATOM	2651	C	ALA	606	67.665	21.770	95.113	1.00	6.88	
ATOM	2652	O	ALA	606	67.450	22.974	95.234	1.00	7.80	
ATOM	2653	N	PRO	607	67.222	21.063	94.074	1.00	6.21	
ATOM	2654	CD	PRO	607	67.457	19.636	93.821	1.00	6.78	
ATOM	2655	CA	PRO	607	66.520	21.660	92.950	1.00	7.75	
ATOM	2656	CB	PRO	607	66.656	20.587	91.845	1.00	7.27	
ATOM	2657	CG	PRO	607	67.655	19.620	92.355	1.00	5.40	
ATOM	2658	C	PRO	607	65.046	21.969	93.220	1.00	6.86	
ATOM	2659	O	PRO	607	64.287	21.084	93.599	1.00	6.25	
ATOM	2660	N	ARG	608	64.656	23.215	92.953	1.00	6.55	
ATOM	2661	CA	ARG	608	63.284	23.658	93.095	1.00	6.82	
ATOM	2662	CB	ARG	608	63.198	25.105	93.591	1.00	7.55	
ATOM	2663	CG	ARG	608	63.510	25.320	95.066	1.00	11.99	
ATOM	2664	CD	ARG	608	62.608	24.474	95.992	1.00	14.22	
ATOM	2665	NE	ARG	608	61.169	24.719	95.820	1.00	14.28	
ATOM	2666	CZ	ARG	608	60.530	25.828	96.200	1.00	14.39	
ATOM	2667	NH1	ARG	608	61.193	26.817	96.773	1.00	15.96	
ATOM	2668	NH2	ARG	608	59.216	25.936	96.048	1.00	13.38	
ATOM	2669	C	ARG	608	62.586	23.548	91.739	1.00	6.91	
ATOM	2670	O	ARG	608	61.613	22.836	91.612	1.00	8.99	
ATOM	2671	N	TYR	609	63.095	24.194	90.700	1.00	7.03	
ATOM	2672	CA	TYR	609	62.405	24.140	89.406	1.00	7.62	
ATOM	2673	CB	TYR	609	61.532	25.394	89.203	1.00	9.92	
ATOM	2674	CG	TYR	609	60.543	25.684	90.298	1.00	11.75	
ATOM	2675	CD1	TYR	609	60.700	26.798	91.137	1.00	12.36	
ATOM	2676	CE1	TYR	609	59.768	27.078	92.156	1.00	13.98	
ATOM	2677	CD2	TYR	609	59.434	24.852	90.499	1.00	13.86	
ATOM	2678	CE2	TYR	609	58.494	25.120	91.506	1.00	13.63	
ATOM	2679	CZ	TYR	609	58.664	26.235	92.326	1.00	15.21	
ATOM	2680	OH	TYR	609	57.689	26.529	93.255	1.00	17.36	
ATOM	2681	C	TYR	609	63.316	24.032	88.193	1.00	7.45	
ATOM	2682	O	TYR	609	64.448	24.514	88.207	1.00	10.10	
ATOM	2683	N	HIS	610	62.803	23.416	87.137	1.00	4.17	
ATOM	2684	CA	HIS	610	63.536	23.308	85.886	1.00	3.51	
ATOM	2685	CB	HIS	610	64.306	21.995	85.775	1.00	2.85	
ATOM	2686	CG	HIS	610	65.212	21.883	84.524	1.00	2.00	
ATOM	2687	CD2	HIS	610	65.692	22.830	83.753	1.00	2.00	
ATOM	2688	ND1	HIS	610	65.346	20.681	83.896	1.00	2.00	
ATOM	2689	CE1	HIS	610	66.030	20.893	82.786	1.00	2.00	
ATOM	2690	NE2	HIS	610	66.250	22.189	82.676	1.00	2.00	
ATOM	2691	C	HIS	610	62.500	23.456	84.774	1.00	3.94	
ATOM	2692	O	HIS	610	61.459	22.824	84.794	1.00	4.37	
ATOM	2693	N	ARG	611	62.790	24.306	83.807	1.00	4.10	
ATOM	2694	CA	ARG	611	61.858	24.561	82.756	1.00	2.00	
ATOM	2695	CB	ARG	611	60.948	25.703	83.222	1.00	2.00	
ATOM	2696	CG	ARG	611	59.476	25.573	82.826	1.00	5.34	
ATOM	2697	CD	ARG	611	58.701	26.890	82.920	1.00	2.76	
ATOM	2698	NE	ARG	611	57.501	26.833	82.093	1.00	4.99	
ATOM	2699	CZ	ARG	611	56.647	27.834	81.931	1.00	4.31	
ATOM	2700	NH1	ARG	611	56.850	28.973	82.542	1.00	9.07	
ATOM	2701	NH2	ARG	611	55.605	27.711	81.138	1.00	2.00	
ATOM	2702	C	ARG	611	62.657	24.994	81.558	1.00	2.00	
ATOM	2703	O	ARG	611	63.800	25.350	81.680	1.00	3.11	
ATOM	2704	N	VAL	612	62.074	24.833	80.388	1.00	2.76	
ATOM	2705	CA	VAL	612	62.669	25.256	79.118	1.00	5.17	
ATOM	2706	CB	VAL	612	63.056	24.068	78.198	1.00	5.26	
ATOM	2707	CG1	VAL	612	63.806	24.567	76.967	1.00	6.96	
ATOM	2708	CG2	VAL	612	63.917	23.089	78.935	1.00	9.67	
ATOM	2709	C	VAL	612	61.490	25.968	78.464	1.00	4.40	
ATOM	2710	O	VAL	612	60.382	25.436	78.481	1.00	5.97	
ATOM	2711	N	ILE	613	61.674	27.187	77.968	1.00	2.39	
ATOM	2712	CA	ILE	613	60.557	27.874	77.340	1.00	2.00	
ATOM	2713	CB	ILE	613	59.889	28.933	78.270	1.00	2.00	
ATOM	2714	CG2	ILE	613	59.244	28.279	79.471	1.00	2.16	
ATOM	2715	CG1	ILE	613	60.890	30.015	78.669	1.00	2.00	
ATOM	2716	CD1	ILE	613	60.267	31.241	79.182	1.00	2.08	
ATOM	2717	C	ILE	613	60.998	28.601	76.094	1.00	3.35	
ATOM	2718	O	ILE	613	62.164	28.553	75.709	1.00	2.06	
ATOM	2719	N	HIS	614	60.013	29.173	75.412	1.00	3.35	
ATOM	2720	CA	HIS	614	60.252	30.002	74.241	1.00	4.63	
ATOM	2721	CB	HIS	614	59.604	29.427	72.970	1.00	2.35	
ATOM	2722	CG	HIS	614	60.447	28.419	72.271	1.00	2.10	

ATOM	2723	CD2	HIS	614	61.353	28.536	71.281	1.00	2.96	
ATOM	2724	ND1	HIS	614	60.442	27.075	72.609	1.00	4.63	
ATOM	2725	CE1	HIS	614	61.310	26.419	71.865	1.00	2.00	
ATOM	2726	NE2	HIS	614	61.875	27.284	71.051	1.00	6.31	
ATOM	2727	C	HIS	614	59.580	31.311	74.664	1.00	3.58	
ATOM	2728	O	HIS	614	58.419	31.306	75.046	1.00	2.50	
ATOM	2729	N	ILE	615	60.315	32.412	74.674	1.00	2.76	
ATOM	2730	CA	ILE	615	59.717	33.661	75.108	1.00	2.55	
ATOM	2731	CB	ILE	615	60.770	34.768	75.221	1.00	2.49	
ATOM	2732	CG2	ILE	615	60.102	36.115	75.507	1.00	2.99	
ATOM	2733	CG1	ILE	615	61.785	34.387	76.307	1.00	2.00	
ATOM	2734	CD1	ILE	615	63.067	35.246	76.351	1.00	2.00	
ATOM	2735	C	ILE	615	58.569	34.079	74.205	1.00	3.27	
ATOM	2736	O	ILE	615	57.609	34.687	74.651	1.00	5.04	
ATOM	2737	N	ASN	616	58.639	33.673	72.943	1.00	5.73	
ATOM	2738	CA	ASN	616	57.618	34.015	71.945	1.00	4.76	
ATOM	2739	CB	ASN	616	58.205	33.893	70.513	1.00	2.00	
ATOM	2740	CG	ASN	616	58.860	32.539	70.236	1.00	2.00	
ATOM	2741	OD1	ASN	616	58.410	31.767	69.399	1.00	2.00	
ATOM	2742	ND2	ASN	616	59.954	32.273	70.910	1.00	2.00	
ATOM	2743	C	ASN	616	56.287	33.247	72.124	1.00	4.60	
ATOM	2744	O	ASN	616	55.265	33.632	71.581	1.00	6.70	
ATOM	2745	N	GLU	617	56.280	32.240	72.989	1.00	4.63	
ATOM	2746	CA	GLU	617	55.088	31.444	73.242	1.00	5.16	
ATOM	2747	CB	GLU	617	55.424	29.951	73.185	1.00	4.92	
ATOM	2748	CG	GLU	617	56.381	29.633	72.086	1.00	8.53	
ATOM	2749	CD	GLU	617	56.432	28.180	71.704	1.00	11.83	
ATOM	2750	OE1	GLU	617	56.653	27.922	70.498	1.00	15.40	
ATOM	2751	OE2	GLU	617	56.276	27.297	72.575	1.00	14.68	
ATOM	2752	C	GLU	617	54.438	31.744	74.587	1.00	4.18	
ATOM	2753	O	GLU	617	53.440	31.127	74.930	1.00	7.74	
ATOM	2754	N	VAL	618	54.995	32.667	75.354	1.00	3.63	
ATOM	2755	CA	VAL	618	54.433	32.988	76.655	1.00	2.00	
ATOM	2756	CB	VAL	618	55.365	32.566	77.870	1.00	2.00	
ATOM	2757	CG1	VAL	618	55.666	31.109	77.838	1.00	2.00	
ATOM	2758	CG2	VAL	618	56.651	33.337	77.890	1.00	2.00	
ATOM	2759	C	VAL	618	54.119	34.459	76.727	1.00	2.00	
ATOM	2760	O	VAL	618	54.600	35.167	77.616	1.00	2.77	
ATOM	2761	N	VAL	619	53.333	34.937	75.778	1.00	2.00	
ATOM	2762	CA	VAL	619	52.970	36.345	75.792	1.00	3.10	
ATOM	2763	CB	VAL	619	52.765	36.886	74.407	1.00	2.32	
ATOM	2764	CG1	VAL	619	52.741	38.409	74.449	1.00	2.43	
ATOM	2765	CG2	VAL	619	53.884	36.412	73.519	1.00	7.61	
ATOM	2766	C	VAL	619	51.700	36.587	76.589	1.00	4.11	
ATOM	2767	O	VAL	619	50.817	35.731	76.610	1.00	6.41	
ATOM	2768	N	LEU	620	51.639	37.734	77.268	1.00	2.53	
ATOM	2769	CA	LEU	620	50.492	38.143	78.080	1.00	3.37	
ATOM	2770	CB	LEU	620	50.702	37.790	79.554	1.00	3.99	
ATOM	2771	CG	LEU	620	49.613	37.183	80.438	1.00	3.95	
ATOM	2772	CD1	LEU	620	50.233	37.141	81.775	1.00	5.62	
ATOM	2773	CD2	LEU	620	48.306	37.985	80.529	1.00	3.21	
ATOM	2774	C	LEU	620	50.382	39.654	77.920	1.00	5.44	
ATOM	2775	O	LEU	620	50.858	40.437	78.736	1.00	7.07	
ATOM	2776	N	LEU	621	49.739	40.044	76.834	1.00	7.07	
ATOM	2777	CA	LEU	621	49.549	41.432	76.465	1.00	5.70	
ATOM	2778	CB	LEU	621	48.832	41.498	75.111	1.00	5.58	
ATOM	2779	CG	LEU	621	49.469	40.971	73.845	1.00	2.00	
ATOM	2780	CD1	LEU	621	48.395	40.832	72.831	1.00	2.42	
ATOM	2781	CD2	LEU	621	50.545	41.903	73.377	1.00	2.00	
ATOM	2782	C	LEU	621	48.730	42.253	77.427	1.00	7.59	
ATOM	2783	O	LEU	621	47.941	41.728	78.198	1.00	8.04	
ATOM	2784	N	ASP	622	48.928	43.565	77.355	1.00	11.43	
ATOM	2785	CA	ASP	622	48.148	44.513	78.128	1.00	10.55	
ATOM	2786	CB	ASP	622	48.678	45.938	77.968	1.00	9.98	
ATOM	2787	CG	ASP	622	49.746	46.300	78.963	1.00	11.16	
ATOM	2788	OD1	ASP	622	50.398	47.342	78.724	1.00	12.42	
ATOM	2789	OD2	ASP	622	49.927	45.580	79.976	1.00	11.12	
ATOM	2790	C	ASP	622	46.855	44.429	77.336	1.00	10.98	
ATOM	2791	O	ASP	622	46.867	44.075	76.152	1.00	11.16	
ATOM	2792	N	ALA	623	45.754	44.808	77.965	1.00	13.11	
ATOM	2793	CA	ALA	623	44.452	44.764	77.326	1.00	12.49	
ATOM	2794	CB	ALA	623	43.375	44.723	78.402	1.00	13.24	
ATOM	2795	C	ALA	623	44.267	45.975	76.399	1.00	10.77	
ATOM	2796	O	ALA	623	45.013	46.953	76.489	1.00	11.43	
ATOM	2797	N	PRO	624	43.311	45.890	75.462	1.00	7.62	
ATOM	2798	CD	PRO	624	42.607	44.628	75.175	1.00	7.09	
ATOM	2799	CA	PRO	624	42.969	46.928	74.486	1.00	6.69	
ATOM	2800	CB	PRO	624	41.933	46.241	73.632	1.00	6.32	

ATOM	2801	CG	PRO	624	42.334	44.750	73.736	1.00	9.96	
ATOM	2802	C	PRO	624	42.366	48.198	75.095	1.00	10.98	
ATOM	2803	O	PRO	624	41.591	48.139	76.056	1.00	13.90	
ATOM	2804	N	VAL	625	42.693	49.352	74.518	1.00	11.27	
ATOM	2805	CA	VAL	625	42.152	50.638	74.969	1.00	8.57	
ATOM	2806	CB	VAL	625	43.254	51.676	75.160	1.00	8.17	
ATOM	2807	CG1	VAL	625	44.097	51.324	76.386	1.00	10.17	
ATOM	2808	CG2	VAL	625	44.116	51.744	73.933	1.00	6.41	
ATOM	2809	C	VAL	625	41.136	51.193	73.950	1.00	11.00	
ATOM	2810	O	VAL	625	40.779	50.513	72.970	1.00	11.35	
ATOM	2811	N	GLY	626	40.629	52.392	74.243	1.00	10.53	
ATOM	2812	CA	GLY	626	39.683	53.098	73.389	1.00	12.11	
ATOM	2813	C	GLY	626	38.396	52.482	72.843	1.00	14.18	
ATOM	2814	O	GLY	626	37.906	52.907	71.775	1.00	14.32	
ATOM	2815	N	LEU	627	37.819	51.522	73.565	1.00	16.06	
ATOM	2816	CA	LEU	627	36.576	50.879	73.112	1.00	17.03	
ATOM	2817	CB	LEU	627	36.138	49.789	74.092	1.00	13.89	
ATOM	2818	CG	LEU	627	34.946	48.955	73.631	1.00	13.26	
ATOM	2819	CD1	LEU	627	35.399	48.124	72.467	1.00	15.73	
ATOM	2820	CD2	LEU	627	34.421	48.034	74.740	1.00	12.93	
ATOM	2821	C	LEU	627	35.415	51.869	72.928	1.00	18.27	
ATOM	2822	O	LEU	627	35.007	52.548	73.881	1.00	17.62	
ATOM	2823	N	VAL	628	34.954	52.005	71.682	1.00	19.54	
ATOM	2824	CA	VAL	628	33.814	52.862	71.355	1.00	19.76	
ATOM	2825	CB	VAL	628	34.166	54.119	70.490	1.00	18.01	
ATOM	2826	CG1	VAL	628	34.935	55.151	71.318	1.00	19.05	
ATOM	2827	CG2	VAL	628	34.942	53.723	69.244	1.00	18.46	
ATOM	2828	C	VAL	628	32.787	52.009	70.609	1.00	21.07	
ATOM	2829	O	VAL	628	33.146	51.171	69.740	1.00	19.35	
ATOM	2830	N	ALA	629	31.528	52.157	71.036	1.00	21.23	
ATOM	2831	CA	ALA	629	30.393	51.453	70.440	1.00	21.69	
ATOM	2832	CB	ALA	629	29.532	50.850	71.531	1.00	25.97	
ATOM	2833	C	ALA	629	29.593	52.496	69.664	1.00	22.67	
ATOM	2834	O	ALA	629	29.684	53.693	69.980	1.00	23.69	
ATOM	2835	N	ARG	630	28.823	52.061	68.659	1.00	22.36	
ATOM	2836	CA	ARG	630	28.014	52.979	67.845	1.00	19.90	
ATOM	2837	CB	ARG	630	28.813	53.703	66.809	1.00	19.83	
ATOM	2838	CG	ARG	630	29.087	55.154	67.175	1.00	22.67	
ATOM	2839	CD	ARG	630	29.565	56.016	65.999	1.00	24.86	
ATOM	2840	NE	ARG	630	29.366	57.461	66.223	1.00	26.19	
ATOM	2841	CZ	ARG	630	29.627	58.112	67.368	1.00	28.04	
ATOM	2842	NH1	ARG	630	30.108	57.460	68.455	1.00	26.78	
ATOM	2843	NH2	ARG	630	29.421	59.440	67.426	1.00	26.78	
ATOM	2844	C	ARG	630	26.867	52.308	67.125	1.00	19.88	
ATOM	2845	O	ARG	630	26.945	51.133	66.764	1.00	19.93	
ATOM	2846	N	LEU	631	25.787	53.049	66.944	1.00	18.72	
ATOM	2847	CA	LEU	631	24.650	52.498	66.238	1.00	18.88	
ATOM	2848	CB	LEU	631	23.379	53.267	66.602	1.00	18.29	
ATOM	2849	CG	LEU	631	22.269	52.408	67.214	1.00	17.34	
ATOM	2850	CD1	LEU	631	22.275	50.967	66.721	1.00	18.01	
ATOM	2851	CD2	LEU	631	22.351	52.322	68.740	1.00	18.98	
ATOM	2852	C	LEU	631	24.826	52.770	64.791	1.00	21.02	
ATOM	2853	O	LEU	631	24.739	53.915	64.341	1.00	23.22	
ATOM	2854	N	ALA	632	25.094	51.758	64.057	1.00	21.42	
ATOM	2855	CA	ALA	632	25.170	51.975	62.641	1.00	22.08	
ATOM	2856	CB	ALA	632	25.601	50.699	61.943	1.00	23.97	
ATOM	2857	C	ALA	632	23.771	52.420	62.235	1.00	24.54	
ATOM	2858	O	ALA	632	22.964	51.604	61.790	1.00	25.46	
ATOM	2859	N	ASP	633	23.542	53.700	62.434	1.00	90.00	
ATOM	2860	CA	ASP	633	22.239	54.366	62.208	1.00	90.00	
ATOM	2861	CB	ASP	633	22.438	55.880	62.013	1.00	90.00	
ATOM	2862	CG	ASP	633	22.352	56.775	63.273	1.00	90.00	
ATOM	2863	OD1	ASP	633	21.778	56.363	64.347	1.00	90.00	
ATOM	2864	OD2	ASP	633	22.852	57.977	63.227	1.00	90.00	
ATOM	2865	C	ASP	633	21.466	53.894	60.821	1.00	90.00	
ATOM	2866	O	ASP	633	20.253	53.666	60.947	1.00	90.00	
ATOM	2867	N	GLU	634	22.137	53.747	59.752	1.00	90.00	
ATOM	2868	CA	GLU	634	21.428	53.465	58.504	1.00	90.00	
ATOM	2869	CB	GLU	634	22.349	53.756	57.325	1.00	90.00	
ATOM	2870	CG	GLU	634	22.847	55.203	57.327	1.00	90.00	
ATOM	2871	CD	GLU	634	23.766	55.525	56.151	1.00	90.00	
ATOM	2872	OE1	GLU	634	24.012	54.625	55.261	1.00	90.00	
ATOM	2873	OE2	GLU	634	24.295	56.697	56.049	1.00	90.00	
ATOM	2874	C	GLU	634	20.911	52.021	58.373	1.00	90.00	
ATOM	2875	O	GLU	634	20.024	51.726	57.583	1.00	90.00	
ATOM	2876	N	SER	635	21.465	51.135	59.168	1.00	90.00	
ATOM	2877	CA	SER	635	21.062	49.720	59.145	1.00	90.00	
ATOM	2878	CB	SER	635	22.288	48.820	58.994	1.00	90.00	

bref21c.pdb Thu Apr 25 12:27:47 1996 38

ATOM	2879	OG	SER	635	23.189	49.037	60.063	1.00	90.00
ATOM	2880	C	SER	635	20.328	49.370	60.435	1.00	90.00
ATOM	2881	O	SER	635	19.394	48.552	60.427	1.00	90.00
ATOM	2882	N	GLY	636	20.780	50.010	61.468	1.00	90.00
ATOM	2883	CA	GLY	636	20.217	49.834	62.821	1.00	90.00
ATOM	2884	C	GLY	636	20.996	48.771	63.586	1.00	90.00
ATOM	2885	O	GLY	636	20.541	47.640	63.790	1.00	90.00
ATOM	2886	N	HIS	637	22.203	49.107	64.010	1.00	29.39
ATOM	2887	CA	HIS	637	22.920	48.155	64.847	1.00	28.30
ATOM	2888	CB	HIS	637	23.190	46.817	64.148	1.00	27.49
ATOM	2889	CG	HIS	637	23.915	46.854	62.796	1.00	26.32
ATOM	2890	CD2	HIS	637	25.124	47.337	62.400	1.00	26.14
ATOM	2891	ND1	HIS	637	23.338	46.289	61.665	1.00	26.56
ATOM	2892	CE1	HIS	637	24.176	46.428	60.659	1.00	26.93
ATOM	2893	NE2	HIS	637	25.247	47.050	61.079	1.00	26.35
ATOM	2894	C	HIS	637	24.223	48.651	65.427	1.00	27.39
ATOM	2895	O	HIS	637	24.505	49.862	65.452	1.00	27.46
ATOM	2896	N	VAL	638	24.921	47.631	65.868	1.00	25.98
ATOM	2897	CA	VAL	638	26.119	47.770	66.646	1.00	22.67
ATOM	2898	CB	VAL	638	26.169	46.693	67.730	1.00	23.93
ATOM	2899	CG1	VAL	638	26.966	47.127	68.963	1.00	24.68
ATOM	2900	CG2	VAL	638	24.781	46.310	68.251	1.00	23.20
ATOM	2901	C	VAL	638	27.422	47.694	65.877	1.00	21.16
ATOM	2902	O	VAL	638	27.763	46.687	65.236	1.00	17.80
ATOM	2903	N	VAL	639	28.129	48.808	65.940	1.00	19.71
ATOM	2904	CA	VAL	639	29.417	48.927	65.309	1.00	21.49
ATOM	2905	CB	VAL	639	29.362	49.967	64.127	1.00	22.97
ATOM	2906	CG1	VAL	639	30.383	51.140	64.296	1.00	22.32
ATOM	2907	CG2	VAL	639	29.531	49.189	62.796	1.00	21.09
ATOM	2908	C	VAL	639	30.503	49.131	66.402	1.00	18.72
ATOM	2909	O	VAL	639	30.569	50.164	67.103	1.00	15.61
ATOM	2910	N	LEU	640	31.245	48.035	66.588	1.00	17.29
ATOM	2911	CA	LEU	640	32.312	47.853	67.567	1.00	15.07
ATOM	2912	CB	LEU	640	32.296	46.385	68.002	1.00	11.06
ATOM	2913	CG	LEU	640	31.948	45.925	69.398	1.00	9.33
ATOM	2914	CD1	LEU	640	30.755	46.635	69.940	1.00	6.96
ATOM	2915	CD2	LEU	640	31.703	44.456	69.328	1.00	7.60
ATOM	2916	C	LEU	640	33.727	48.158	67.106	1.00	15.19
ATOM	2917	O	LEU	640	34.319	47.345	66.393	1.00	13.52
ATOM	2918	N	ARG	641	34.320	49.236	67.616	1.00	16.40
ATOM	2919	CA	ARG	641	35.717	49.564	67.269	1.00	18.02
ATOM	2920	CB	ARG	641	35.744	50.820	66.406	1.00	18.96
ATOM	2921	CG	ARG	641	36.505	50.608	65.100	1.00	23.80
ATOM	2922	CD	ARG	641	35.742	51.114	63.884	1.00	25.92
ATOM	2923	NE	ARG	641	34.649	50.212	63.502	1.00	26.12
ATOM	2924	CZ	ARG	641	33.446	50.620	63.085	1.00	27.21
ATOM	2925	NH1	ARG	641	33.173	51.935	63.013	1.00	24.02
ATOM	2926	NH2	ARG	641	32.538	49.716	62.685	1.00	23.76
ATOM	2927	C	ARG	641	36.638	49.707	68.527	1.00	17.87
ATOM	2928	O	ARG	641	36.119	49.879	69.655	1.00	19.51
ATOM	2929	N	TRP	642	37.972	49.598	68.366	1.00	16.84
ATOM	2930	CA	TRP	642	38.925	49.723	69.515	1.00	14.61
ATOM	2931	CB	TRP	642	38.765	48.534	70.453	1.00	13.71
ATOM	2932	CG	TRP	642	39.106	47.243	69.819	1.00	9.75
ATOM	2933	CD2	TRP	642	38.203	46.359	69.133	1.00	10.16
ATOM	2934	CE2	TRP	642	38.926	45.195	68.814	1.00	10.08
ATOM	2935	CE3	TRP	642	36.855	46.438	68.760	1.00	8.27
ATOM	2936	CD1	TRP	642	40.304	46.612	69.860	1.00	7.42
ATOM	2937	NE1	TRP	642	40.208	45.377	69.267	1.00	10.16
ATOM	2938	CZ2	TRP	642	38.345	44.116	68.150	1.00	8.53
ATOM	2939	CZ3	TRP	642	36.289	45.374	68.098	1.00	7.26
ATOM	2940	CH2	TRP	642	37.033	44.225	67.803	1.00	7.13
ATOM	2941	C	TRP	642	40.424	49.824	69.178	1.00	15.14
ATOM	2942	O	TRP	642	40.798	49.704	68.006	1.00	17.51
ATOM	2943	N	LEU	643	41.275	49.982	70.207	1.00	13.07
ATOM	2944	CA	LEU	643	42.747	50.063	70.039	1.00	13.34
ATOM	2945	CB	LEU	643	43.310	51.312	70.676	1.00	9.27
ATOM	2946	CG	LEU	643	42.887	52.627	70.081	1.00	9.05
ATOM	2947	CD1	LEU	643	43.784	53.715	70.583	1.00	7.00
ATOM	2948	CD2	LEU	643	43.013	52.525	68.601	1.00	9.98
ATOM	2949	C	LEU	643	43.508	48.891	70.662	1.00	15.42
ATOM	2950	O	LEU	643	43.096	48.351	71.697	1.00	19.66
ATOM	2951	N	PRO	644	44.645	48.493	70.059	1.00	15.88
ATOM	2952	CD	PRO	644	45.206	49.056	68.817	1.00	15.21
ATOM	2953	CA	PRO	644	45.481	47.381	70.556	1.00	14.66
ATOM	2954	CB	PRO	644	46.485	47.175	69.412	1.00	15.17
ATOM	2955	CG	PRO	644	46.642	48.573	68.867	1.00	15.08
ATOM	2956	C	PRO	644	46.192	47.793	71.851	1.00	11.57

ATOM	2957	O	PRO	644	46.148	48.978	72.209	1.00	12.33	3
ATOM	2958	N	PRO	645	46.806	46.824	72.588	1.00	10.67	7
ATOM	2959	CD	PRO	645	46.832	45.392	72.229	1.00	10.47	5
ATOM	2960	CA	PRO	645	47.530	47.049	73.851	1.00	9.59	5
ATOM	2961	CB	PRO	645	48.279	45.746	74.038	1.00	10.22	5
ATOM	2962	CG	PRO	645	47.321	44.742	73.502	1.00	9.51	5
ATOM	2963	C	PRO	645	48.475	48.178	73.572	1.00	9.51	5
ATOM	2964	O	PRO	645	49.211	48.142	72.605	1.00	11.71	3
ATOM	2965	N	PRO	646	48.433	49.229	74.375	1.00	9.63	7
ATOM	2966	CD	PRO	646	47.682	49.431	75.618	1.00	9.62	5
ATOM	2967	CA	PRO	646	49.334	50.350	74.105	1.00	9.90	5
ATOM	2968	CB	PRO	646	49.004	51.345	75.217	1.00	9.95	5
ATOM	2969	CG	PRO	646	47.619	50.941	75.674	1.00	11.92	6
ATOM	2970	C	PRO	646	50.809	49.956	74.116	1.00	13.01	5
ATOM	2971	O	PRO	646	51.204	48.918	74.679	1.00	14.24	8
ATOM	2972	N	GLU	647	51.620	50.786	73.470	1.00	13.38	7
ATOM	2973	CA	GLU	647	53.043	50.546	73.383	1.00	14.58	5
ATOM	2974	CB	GLU	647	53.753	51.217	74.552	1.00	15.62	5
ATOM	2975	CG	GLU	647	53.788	52.737	74.380	1.00	19.18	6
ATOM	2976	CD	GLU	647	54.239	53.470	75.640	1.00	20.10	6
ATOM	2977	OE1	GLU	647	53.641	53.215	76.715	1.00	22.78	8
ATOM	2978	OE2	GLU	647	55.175	54.305	75.563	1.00	19.41	8
ATOM	2979	C	GLU	647	53.485	49.082	73.218	1.00	14.37	6
ATOM	2980	O	GLU	647	54.508	48.697	73.795	1.00	18.36	8
ATOM	2981	N	THR	648	52.755	48.316	72.384	1.00	11.24	7
ATOM	2982	CA	THR	648	53.029	46.899	72.062	1.00	9.00	5
ATOM	2983	CB	THR	648	51.832	45.984	72.452	1.00	9.78	5
ATOM	2984	OG1	THR	648	51.552	46.119	73.852	1.00	10.70	8
ATOM	2985	CG2	THR	648	52.134	44.533	72.141	1.00	8.04	5
ATOM	2986	C	THR	648	53.295	46.761	70.534	1.00	9.27	5
ATOM	2987	O	THR	648	52.584	47.370	69.715	1.00	9.52	8
ATOM	2988	N	PRO	649	54.320	45.968	70.137	1.00	7.20	7
ATOM	2989	CD	PRO	649	55.333	45.245	70.941	1.00	6.54	6
ATOM	2990	CA	PRO	649	54.610	45.819	68.713	1.00	6.88	5
ATOM	2991	CB	PRO	649	56.106	45.495	68.711	1.00	5.46	6
ATOM	2992	CG	PRO	649	56.233	44.592	69.879	1.00	3.39	6
ATOM	2993	C	PRO	649	53.827	44.707	68.075	1.00	8.17	6
ATOM	2994	O	PRO	649	52.957	44.106	68.705	1.00	9.10	8
ATOM	2995	N	MET	650	54.224	44.406	66.838	1.00	9.01	7
ATOM	2996	CA	MET	650	53.645	43.363	65.987	1.00	9.79	5
ATOM	2997	CB	MET	650	54.158	41.969	66.370	1.00	8.66	6
ATOM	2998	CG	MET	650	55.676	41.834	66.230	1.00	7.85	5
ATOM	2999	SD	MET	650	56.219	41.811	64.535	1.00	7.28	16
ATOM	3000	CE	MET	650	56.577	40.141	64.037	1.00	2.00	5
ATOM	3001	C	MET	650	52.112	43.354	65.975	1.00	11.50	5
ATOM	3002	O	MET	650	51.478	42.289	65.991	1.00	13.41	8
ATOM	3003	N	THR	651	51.581	44.546	65.891	1.00	11.63	7
ATOM	3004	CA	THR	651	50.136	44.808	65.906	1.00	12.15	5
ATOM	3005	CB	THR	651	49.858	46.198	65.323	1.00	13.04	5
ATOM	3006	OG1	THR	651	50.419	47.197	66.162	1.00	14.67	5
ATOM	3007	CG2	THR	651	48.364	46.502	65.187	1.00	15.74	5
ATOM	3008	C	THR	651	49.353	43.784	65.039	1.00	12.51	5
ATOM	3009	O	THR	651	48.309	43.264	65.454	1.00	16.75	8
ATOM	3010	N	SER	652	49.866	43.478	63.829	1.00	11.13	7
ATOM	3011	CA	SER	652	49.110	42.623	62.863	1.00	6.89	5
ATOM	3012	CB	SER	652	49.510	42.949	61.416	1.00	5.16	5
ATOM	3013	OG	SER	652	50.405	41.990	60.895	1.00	4.04	8
ATOM	3014	C	SER	652	49.235	41.114	63.151	1.00	7.54	5
ATOM	3015	O	SER	652	49.034	40.261	62.274	1.00	9.34	8
ATOM	3016	N	HIS	653	49.523	40.795	64.390	1.00	7.77	7
ATOM	3017	CA	HIS	653	49.584	39.399	64.805	1.00	6.49	5
ATOM	3018	CB	HIS	653	50.991	39.071	65.253	1.00	6.61	5
ATOM	3019	CG	HIS	653	51.892	38.953	64.029	1.00	9.79	8
ATOM	3020	CD2	HIS	653	52.285	37.884	63.288	1.00	9.28	7
ATOM	3021	ND1	HIS	653	52.471	40.071	63.438	1.00	10.33	7
ATOM	3022	CE1	HIS	653	53.171	39.668	62.395	1.00	9.42	5
ATOM	3023	NE2	HIS	653	53.071	38.367	62.291	1.00	7.91	7
ATOM	3024	C	HIS	653	48.476	39.163	65.830	1.00	4.62	5
ATOM	3025	O	HIS	653	47.989	38.044	65.994	1.00	5.90	8
ATOM	3026	N	ILE	654	48.046	40.234	66.470	1.00	5.11	7
ATOM	3027	CA	ILE	654	47.072	40.145	67.580	1.00	4.75	5
ATOM	3028	CB	ILE	654	47.059	41.456	68.355	1.00	3.95	5
ATOM	3029	CG2	ILE	654	46.252	41.368	69.653	1.00	5.93	5
ATOM	3030	CG1	ILE	654	48.469	41.891	68.760	1.00	3.24	5
ATOM	3031	CD1	ILE	654	48.560	43.367	69.131	1.00	2.00	5
ATOM	3032	C	ILE	654	45.633	39.787	67.156	1.00	5.10	5
ATOM	3033	O	ILE	654	44.981	40.508	66.395	1.00	7.39	8
ATOM	3034	N	ARG	655	45.214	38.661	67.713	1.00	5.70	7

bref21c.pdb Thu Apr 25 12:27:47 1996 40

```
ATOM   3035  CA  ARG   655      43.856  38.107  67.582  1.00  4.70      6
ATOM   3036  CB  ARG   655      43.947  36.608  67.851  1.00  6.54      6
ATOM   3037  CG  ARG   655      42.732  35.835  67.393  1.00 12.78      6
ATOM   3038  CD  ARG   655      42.923  35.234  66.013  1.00 19.16      6
ATOM   3039  NE  ARG   655      41.690  35.243  65.243  1.00 25.22      7
ATOM   3040  CZ  ARG   655      41.487  34.509  64.155  1.00 28.18      6
ATOM   3041  NH1 ARG   655      42.441  33.699  63.683  1.00 29.93      7
ATOM   3042  NH2 ARG   655      40.343  34.523  63.465  1.00 30.11      7
ATOM   3043  C   ARG   655      43.012  38.786  68.687  1.00  4.93      6
ATOM   3044  O   ARG   655      43.561  39.225  69.706  1.00  4.78      8
ATOM   3045  N   TYR   656      41.706  38.916  68.485  1.00  3.05      7
ATOM   3046  CA  TYR   656      40.852  39.533  69.491  1.00  4.57      6
ATOM   3047  CB  TYR   656      40.315  40.886  69.041  1.00  5.74      6
ATOM   3048  CG  TYR   656      41.339  41.973  69.131  1.00 11.08      6
ATOM   3049  CD1 TYR   656      41.994  42.423  67.995  1.00 11.86      6
ATOM   3050  CE1 TYR   656      43.029  43.341  68.077  1.00 13.79      6
ATOM   3051  CD2 TYR   656      41.736  42.482  70.366  1.00 13.83      6
ATOM   3052  CE2 TYR   656      42.779  43.407  70.461  1.00 14.75      6
ATOM   3053  CZ  TYR   656      43.422  43.826  69.307  1.00 14.26      6
ATOM   3054  OH  TYR   656      44.498  44.701  69.373  1.00 19.33      8
ATOM   3055  C   TYR   656      39.693  38.646  69.848  1.00  7.31      6
ATOM   3056  O   TYR   656      39.504  37.608  69.210  1.00  7.58      8
ATOM   3057  N   GLU   657      38.967  39.048  70.905  1.00  9.63      7
ATOM   3058  CA  GLU   657      37.776  38.359  71.431  1.00  9.06      6
ATOM   3059  CB  GLU   657      38.109  37.385  72.555  1.00 11.39      6
ATOM   3060  CG  GLU   657      36.874  36.766  73.217  1.00 14.76      6
ATOM   3061  CD  GLU   657      36.755  35.254  72.977  1.00 17.29      6
ATOM   3062  OE1 GLU   657      36.157  34.838  71.945  1.00 19.32      8
ATOM   3063  OE2 GLU   657      37.245  34.472  73.826  1.00 18.57      8
ATOM   3064  C   GLU   657      36.827  39.366  72.006  1.00 10.04      6
ATOM   3065  O   GLU   657      37.163  40.033  72.985  1.00  8.78      8
ATOM   3066  N   VAL   658      35.635  39.428  71.412  1.00 13.32      7
ATOM   3067  CA  VAL   658      34.550  40.334  71.819  1.00 15.04      6
ATOM   3068  CB  VAL   658      33.826  40.908  70.578  1.00 17.13      6
ATOM   3069  CG1 VAL   658      32.355  41.228  70.903  1.00 18.15      6
ATOM   3070  CG2 VAL   658      34.552  42.151  70.055  1.00 15.29      6
ATOM   3071  C   VAL   658      33.518  39.602  72.697  1.00 15.57      6
ATOM   3072  O   VAL   658      33.025  38.519  72.336  1.00 16.39      8
ATOM   3073  N   ASP   659      33.168  40.225  73.818  1.00 15.80      7
ATOM   3074  CA  ASP   659      32.217  39.660  74.762  1.00 16.22      6
ATOM   3075  CB  ASP   659      32.857  39.583  76.152  1.00 18.33      6
ATOM   3076  CG  ASP   659      31.841  39.320  77.262  1.00 17.02      6
ATOM   3077  OD1 ASP   659      31.706  40.220  78.127  1.00 16.96      8
ATOM   3078  OD2 ASP   659      31.191  38.238  77.248  1.00 15.05      8
ATOM   3079  C   ASP   659      30.959  40.488  74.877  1.00 17.09      6
ATOM   3080  O   ASP   659      30.946  41.480  75.641  1.00 16.55      8
ATOM   3081  N   VAL   660      29.924  40.096  74.127  1.00 17.40      7
ATOM   3082  CA  VAL   660      28.623  40.775  74.150  1.00 18.10      6
ATOM   3083  CB  VAL   660      27.835  40.550  72.857  1.00 15.37      6
ATOM   3084  CG1 VAL   660      28.760  40.397  71.683  1.00 16.34      6
ATOM   3085  CG2 VAL   660      26.931  39.368  72.990  1.00 15.04      6
ATOM   3086  C   VAL   660      27.768  40.299  75.335  1.00 20.40      6
ATOM   3087  O   VAL   660      27.719  39.092  75.635  1.00 21.69      8
ATOM   3088  N   SER   661      27.018  41.218  75.943  1.00 22.33      7
ATOM   3089  CA  SER   661      26.210  40.865  77.104  1.00 23.37      6
ATOM   3090  CB  SER   661      27.146  40.683  78.308  1.00 23.56      6
ATOM   3091  OG  SER   661      28.007  39.569  78.169  1.00 25.08      8
ATOM   3092  C   SER   661      25.132  41.882  77.544  1.00 25.29      6
ATOM   3093  O   SER   661      24.814  42.901  76.839  1.00 24.57      8
ATOM   3094  N   ALA   662      24.676  41.596  78.784  1.00 26.02      7
ATOM   3095  CA  ALA   662      23.690  42.325  79.598  1.00 23.48      6
ATOM   3096  CB  ALA   662      23.909  43.856  79.493  1.00 24.66      6
ATOM   3097  C   ALA   662      22.242  41.933  79.339  1.00 22.08      6
ATOM   3098  O   ALA   662      21.935  40.739  79.266  1.00 16.69      8
ATOM   3099  N   GLY   663      21.367  42.948  79.300  1.00 23.15      7
ATOM   3100  CA  GLY   663      19.936  42.775  79.047  1.00 24.87      6
ATOM   3101  C   GLY   663      19.124  41.953  80.038  1.00 23.53      6
ATOM   3102  O   GLY   663      18.542  40.929  79.649  1.00 22.72      8
ATOM   3103  N   ASN   664      19.032  42.453  81.277  1.00 24.09      7
ATOM   3104  CA  ASN   664      18.317  41.816  82.410  1.00 25.66      6
ATOM   3105  CB  ASN   664      17.157  42.706  82.938  1.00 27.33      6
ATOM   3106  CG  ASN   664      15.907  42.725  82.013  1.00 28.05      6
ATOM   3107  OD1 ASN   664      15.791  43.578  81.214  1.00 29.36      8
ATOM   3108  ND2 ASN   664      14.939  41.852  82.294  1.00 26.86      7
ATOM   3109  C   ASN   664      17.831  40.352  82.334  1.00 25.76      6
ATOM   3110  O   ASN   664      16.976  39.992  81.488  1.00 25.92      8
ATOM   3111  N   GLY   665      18.350  39.517  83.243  1.00 24.45      7
ATOM   3112  CA  GLY   665      17.918  38.123  83.294  1.00 24.29      6
```

ATOM	3113	C	GLY	665	18.560	37.239	82.235	1.00	23.94	6
ATOM	3114	O	GLY	665	18.754	36.011	82.454	1.00	24.01	8
ATOM	3115	N	ALA	666	18.767	37.805	81.047	1.00	22.31	7
ATOM	3116	CA	ALA	666	19.457	37.054	80.035	1.00	22.71	6
ATOM	3117	CB	ALA	666	19.331	37.724	78.693	1.00	21.95	6
ATOM	3118	C	ALA	666	20.893	37.166	80.577	1.00	24.38	6
ATOM	3119	O	ALA	666	21.300	38.225	81.075	1.00	25.18	8
ATOM	3120	N	GLY	667	21.579	36.036	80.672	1.00	25.52	7
ATOM	3121	CA	GLY	667	22.941	36.058	81.159	1.00	26.48	6
ATOM	3122	C	GLY	667	23.838	35.946	79.949	1.00	28.11	6
ATOM	3123	O	GLY	667	24.789	35.145	79.937	1.00	29.47	8
ATOM	3124	N	SER	668	23.483	36.689	78.896	1.00	28.73	7
ATOM	3125	CA	SER	668	24.256	36.669	77.641	1.00	28.04	6
ATOM	3126	CB	SER	668	23.634	37.605	76.547	1.00	28.80	6
ATOM	3127	OG	SER	668	24.312	37.574	75.278	1.00	24.54	8
ATOM	3128	C	SER	668	25.597	37.209	78.057	1.00	27.60	6
ATOM	3129	O	SER	668	25.647	38.220	78.798	1.00	27.37	8
ATOM	3130	N	VAL	669	26.623	36.397	77.762	1.00	26.59	7
ATOM	3131	CA	VAL	669	28.049	36.715	77.987	1.00	23.08	6
ATOM	3132	CB	VAL	669	28.665	35.974	79.266	1.00	20.59	6
ATOM	3133	CG1	VAL	669	28.460	34.484	79.178	1.00	19.42	6
ATOM	3134	CG2	VAL	669	30.175	36.316	79.456	1.00	20.06	6
ATOM	3135	C	VAL	669	28.668	36.266	76.644	1.00	21.55	6
ATOM	3136	O	VAL	669	29.846	35.888	76.545	1.00	20.19	8
ATOM	3137	N	GLN	670	27.845	36.409	75.598	1.00	20.21	7
ATOM	3138	CA	GLN	670	28.193	36.009	74.245	1.00	18.75	6
ATOM	3139	CB	GLN	670	27.005	36.236	73.312	1.00	17.59	6
ATOM	3140	CG	GLN	670	27.182	35.569	71.935	1.00	22.13	6
ATOM	3141	CD	GLN	670	27.933	36.432	70.902	1.00	22.70	6
ATOM	3142	OE1	GLN	670	28.500	37.485	71.234	1.00	24.66	8
ATOM	3143	NE2	GLN	670	27.912	35.995	69.634	1.00	23.69	7
ATOM	3144	C	GLN	670	29.519	36.583	73.696	1.00	17.46	6
ATOM	3145	O	GLN	670	29.792	37.782	73.770	1.00	15.56	8
ATOM	3146	N	ARG	671	30.332	35.679	73.157	1.00	15.69	7
ATOM	3147	CA	ARG	671	31.631	36.013	72.639	1.00	16.60	6
ATOM	3148	CB	ARG	671	32.678	35.334	73.517	1.00	17.57	6
ATOM	3149	CG	ARG	671	32.946	36.061	74.887	1.00	19.96	6
ATOM	3150	CD	ARG	671	32.493	35.269	76.139	1.00	18.73	6
ATOM	3151	NE	ARG	671	32.986	35.894	77.368	1.00	19.78	7
ATOM	3152	CZ	ARG	671	33.863	35.344	78.218	1.00	19.40	6
ATOM	3153	NH1	ARG	671	34.370	34.124	78.021	1.00	17.08	7
ATOM	3154	NH2	ARG	671	34.304	36.062	79.241	1.00	17.95	7
ATOM	3155	C	ARG	671	31.869	35.669	71.158	1.00	18.54	6
ATOM	3156	O	ARG	671	31.425	34.618	70.645	1.00	20.62	8
ATOM	3157	N	VAL	672	32.576	36.556	70.460	1.00	18.18	7
ATOM	3158	CA	VAL	672	32.879	36.337	69.049	1.00	15.30	6
ATOM	3159	CB	VAL	672	32.079	37.317	68.160	1.00	15.97	6
ATOM	3160	CG1	VAL	672	30.649	37.440	68.682	1.00	17.58	6
ATOM	3161	CG2	VAL	672	32.728	38.702	68.133	1.00	17.86	6
ATOM	3162	C	VAL	672	34.379	36.538	68.849	1.00	14.22	6
ATOM	3163	O	VAL	672	34.964	37.495	69.358	1.00	14.18	8
ATOM	3164	N	GLU	673	35.011	35.587	68.184	1.00	13.30	7
ATOM	3165	CA	GLU	673	36.437	35.666	67.911	1.00	14.85	6
ATOM	3166	CB	GLU	673	36.902	34.409	67.150	1.00	17.98	6
ATOM	3167	CG	GLU	673	36.621	34.525	65.601	1.00	21.07	6
ATOM	3168	CD	GLU	673	36.996	33.299	64.759	1.00	22.50	6
ATOM	3169	OE1	GLU	673	36.964	32.153	65.300	1.00	20.19	8
ATOM	3170	OE2	GLU	673	37.279	33.501	63.537	1.00	23.59	8
ATOM	3171	C	GLU	673	36.645	36.859	66.978	1.00	14.79	6
ATOM	3172	O	GLU	673	35.688	37.420	66.456	1.00	15.66	8
ATOM	3173	N	ILE	674	37.899	37.192	66.708	1.00	15.73	7
ATOM	3174	CA	ILE	674	38.224	38.270	65.790	1.00	15.34	6
ATOM	3175	CB	ILE	674	38.340	39.659	66.498	1.00	16.72	6
ATOM	3176	CG2	ILE	674	38.785	40.718	65.483	1.00	15.50	6
ATOM	3177	CG1	ILE	674	37.060	40.044	67.289	1.00	15.11	6
ATOM	3178	CD1	ILE	674	35.824	40.386	66.489	1.00	12.07	6
ATOM	3179	C	ILE	674	39.596	37.922	65.198	1.00	16.94	6
ATOM	3180	O	ILE	674	40.511	37.502	65.909	1.00	15.56	8
ATOM	3181	N	LEU	675	39.722	38.012	63.884	1.00	18.65	7
ATOM	3182	CA	LEU	675	41.000	37.737	63.251	1.00	16.13	6
ATOM	3183	CB	LEU	675	40.846	37.553	61.744	1.00	16.02	6
ATOM	3184	CG	LEU	675	40.335	36.155	61.359	1.00	17.94	6
ATOM	3185	CD1	LEU	675	38.786	36.050	61.326	1.00	13.53	6
ATOM	3186	CD2	LEU	675	40.967	35.742	60.014	1.00	18.65	6
ATOM	3187	C	LEU	675	41.944	38.895	63.585	1.00	16.58	6
ATOM	3188	O	LEU	675	41.500	40.013	63.920	1.00	16.45	8
ATOM	3189	N	GLU	676	43.240	38.587	63.521	1.00	14.67	7
ATOM	3190	CA	GLU	676	44.316	39.516	63.829	1.00	12.70	6

ATOM	3191	CB	GLU	676	45.667	38.907	63.526	1.00	12.08
ATOM	3192	CG	GLU	676	45.627	37.882	62.478	1.00	11.18
ATOM	3193	CD	GLU	676	45.494	36.518	63.080	1.00	13.77
ATOM	3194	OE1	GLU	676	46.538	36.007	63.546	1.00	16.32
ATOM	3195	OE2	GLU	676	44.367	35.967	63.108	1.00	13.00
ATOM	3196	C	GLU	676	44.268	40.836	63.146	1.00	12.13
ATOM	3197	O	GLU	676	43.569	41.007	62.159	1.00	12.89
ATOM	3198	N	GLY	677	45.030	41.772	63.699	1.00	11.52
ATOM	3199	CA	GLY	677	45.121	43.103	63.145	1.00	11.07
ATOM	3200	C	GLY	677	43.796	43.794	62.961	1.00	11.96
ATOM	3201	O	GLY	677	43.770	44.949	62.523	1.00	14.32
ATOM	3202	N	ARG	678	42.700	43.134	63.329	1.00	12.98
ATOM	3203	CA	ARG	678	41.387	43.743	63.174	1.00	14.43
ATOM	3204	CB	ARG	678	40.342	42.666	62.927	1.00	13.34
ATOM	3205	CG	ARG	678	39.529	42.932	61.695	1.00	15.05
ATOM	3206	CD	ARG	678	40.401	42.681	60.504	1.00	17.70
ATOM	3207	NE	ARG	678	41.014	41.368	60.643	1.00	22.61
ATOM	3208	CZ	ARG	678	41.887	40.845	59.787	1.00	23.28
ATOM	3209	NH1	ARG	678	42.274	41.525	58.700	1.00	22.06
ATOM	3210	NH2	ARG	678	42.380	39.631	60.037	1.00	25.26
ATOM	3211	C	ARG	678	41.001	44.532	64.420	1.00	14.43
ATOM	3212	O	ARG	678	41.199	44.034	65.529	1.00	15.07
ATOM	3213	N	THR	679	40.462	45.743	64.249	1.00	13.15
ATOM	3214	CA	THR	679	40.027	46.552	65.390	1.00	14.13
ATOM	3215	CB	THR	679	40.996	47.685	65.669	1.00	14.19
ATOM	3216	OG1	THR	679	41.204	48.405	64.448	1.00	17.57
ATOM	3217	CG2	THR	679	42.332	47.148	66.229	1.00	13.59
ATOM	3218	C	THR	679	38.637	47.171	65.182	1.00	16.43
ATOM	3219	O	THR	679	38.393	48.336	65.540	1.00	15.23
ATOM	3220	N	GLU	680	37.732	46.384	64.604	1.00	18.09
ATOM	3221	CA	GLU	680	36.358	46.812	64.332	1.00	19.04
ATOM	3222	CB	GLU	680	36.289	47.765	63.128	1.00	18.69
ATOM	3223	CG	GLU	680	36.140	47.101	61.755	1.00	18.32
ATOM	3224	CD	GLU	680	35.086	47.782	60.847	1.00	18.05
ATOM	3225	OE1	GLU	680	34.342	47.032	60.138	1.00	16.53
ATOM	3226	OE2	GLU	680	35.019	49.045	60.825	1.00	14.40
ATOM	3227	C	GLU	680	35.489	45.579	64.076	1.00	21.29
ATOM	3228	O	GLU	680	35.887	44.641	63.364	1.00	22.54
ATOM	3229	N	CYS	681	34.299	45.578	64.654	1.00	22.91
ATOM	3230	CA	CYS	681	33.382	44.462	64.498	1.00	24.61
ATOM	3231	CB	CYS	681	33.617	43.402	65.603	1.00	26.42
ATOM	3232	SG	CYS	681	32.134	42.836	66.606	1.00	26.71
ATOM	3233	C	CYS	681	31.958	45.006	64.540	1.00	24.30
ATOM	3234	O	CYS	681	31.579	45.763	65.448	1.00	23.84
ATOM	3235	N	VAL	682	31.181	44.688	63.517	1.00	21.58
ATOM	3236	CA	VAL	682	29.818	45.174	63.511	1.00	20.10
ATOM	3237	CB	VAL	682	29.433	45.877	62.131	1.00	18.07
ATOM	3238	CG1	VAL	682	30.190	45.270	60.969	1.00	16.40
ATOM	3239	CG2	VAL	682	27.952	45.785	61.867	1.00	17.19
ATOM	3240	C	VAL	682	28.861	44.077	64.001	1.00	17.00
ATOM	3241	O	VAL	682	28.659	43.049	63.342	1.00	15.10
ATOM	3242	N	LEU	683	28.449	44.218	65.258	1.00	17.47
ATOM	3243	CA	LEU	683	27.485	43.294	65.859	1.00	20.70
ATOM	3244	CB	LEU	683	27.326	43.584	67.348	1.00	17.50
ATOM	3245	CG	LEU	683	28.420	43.127	68.299	1.00	13.82
ATOM	3246	CD1	LEU	683	28.201	43.741	69.667	1.00	13.45
ATOM	3247	CD2	LEU	683	28.376	41.638	68.387	1.00	15.36
ATOM	3248	C	LEU	683	26.228	43.730	65.104	1.00	24.03
ATOM	3249	O	LEU	683	25.446	44.610	65.544	1.00	24.27
ATOM	3250	N	SER	684	26.087	43.161	63.914	1.00	25.99
ATOM	3251	CA	SER	684	25.003	43.521	63.028	1.00	26.98
ATOM	3252	CB	SER	684	25.222	42.906	61.629	1.00	31.20
ATOM	3253	OG	SER	684	26.502	43.257	61.067	1.00	36.99
ATOM	3254	C	SER	684	23.614	43.199	63.491	1.00	26.69
ATOM	3255	O	SER	684	22.800	44.105	63.699	1.00	27.76
ATOM	3256	N	ASN	685	23.397	41.945	63.826	1.00	24.94
ATOM	3257	CA	ASN	685	22.049	41.496	64.131	1.00	25.85
ATOM	3258	CB	ASN	685	21.716	40.428	63.083	1.00	27.66
ATOM	3259	CG	ASN	685	22.993	39.749	62.504	1.00	28.61
ATOM	3260	OD1	ASN	685	23.994	40.433	62.186	1.00	26.41
ATOM	3261	ND2	ASN	685	22.972	38.406	62.407	1.00	28.57
ATOM	3262	C	ASN	685	21.748	40.978	65.533	1.00	26.76
ATOM	3263	O	ASN	685	22.271	39.905	65.923	1.00	27.14
ATOM	3264	N	LEU	686	20.899	41.706	66.287	1.00	25.95
ATOM	3265	CA	LEU	686	20.583	41.260	67.649	1.00	24.26
ATOM	3266	CB	LEU	686	21.779	41.525	68.584	1.00	22.44
ATOM	3267	CG	LEU	686	22.718	42.760	68.474	1.00	23.47
ATOM	3268	CD1	LEU	686	23.700	42.849	69.708	1.00	21.84

ATOM	3269	CD2	LEU	686	23.563	42.742	67.173	1.00	20.88	6
ATOM	3270	C	LEU	686	19.233	41.566	68.375	1.00	26.62	6
ATOM	3271	O	LEU	686	18.361	40.669	68.478	1.00	27.06	8
ATOM	3272	N	ARG	687	19.035	42.801	68.858	1.00	25.21	7
ATOM	3273	CA	ARG	687	17.838	43.147	69.636	1.00	21.90	6
ATOM	3274	CB	ARG	687	18.117	42.901	71.113	1.00	21.00	6
ATOM	3275	CG	ARG	687	17.254	41.847	71.745	1.00	18.87	6
ATOM	3276	CD	ARG	687	17.778	40.471	71.410	1.00	20.25	6
ATOM	3277	NE	ARG	687	16.883	39.426	71.911	1.00	23.57	7
ATOM	3278	CZ	ARG	687	16.832	38.188	71.416	1.00	24.78	6
ATOM	3279	NH1	ARG	687	17.636	37.837	70.405	1.00	25.89	7
ATOM	3280	NH2	ARG	687	15.969	37.303	71.908	1.00	23.14	7
ATOM	3281	C	ARG	687	17.358	44.587	69.517	1.00	23.37	6
ATOM	3282	O	ARG	687	17.863	45.369	68.695	1.00	24.06	8
ATOM	3283	N	GLY	688	16.420	44.939	70.407	1.00	23.79	7
ATOM	3284	CA	GLY	688	15.825	46.263	70.434	1.00	22.75	6
ATOM	3285	C	GLY	688	15.583	46.644	71.874	1.00	23.19	6
ATOM	3286	O	GLY	688	15.359	45.760	72.726	1.00	21.67	8
ATOM	3287	N	ARG	689	15.712	47.944	72.154	1.00	23.01	7
ATOM	3288	CA	ARG	689	15.531	48.533	73.500	1.00	23.70	6
ATOM	3289	CB	ARG	689	14.034	48.518	73.902	1.00	22.81	6
ATOM	3290	CG	ARG	689	13.543	49.819	74.581	1.00	20.45	6
ATOM	3291	CD	ARG	689	13.398	50.988	73.575	1.00	18.41	6
ATOM	3292	NE	ARG	689	14.071	52.266	73.908	1.00	17.79	7
ATOM	3293	CZ	ARG	689	14.201	52.828	75.128	1.00	19.24	6
ATOM	3294	NH1	ARG	689	13.738	52.253	76.250	1.00	12.88	7
ATOM	3295	NH2	ARG	689	14.704	54.066	75.213	1.00	18.71	7
ATOM	3296	C	ARG	689	16.425	47.958	74.648	1.00	25.87	6
ATOM	3297	O	ARG	689	16.512	48.542	75.756	1.00	25.28	8
ATOM	3298	N	THR	690	17.153	46.887	74.313	1.00	25.78	7
ATOM	3299	CA	THR	690	18.053	46.127	75.182	1.00	23.94	6
ATOM	3300	CB	THR	690	18.530	44.902	74.403	1.00	24.95	6
ATOM	3301	OG1	THR	690	17.550	44.550	73.405	1.00	24.96	8
ATOM	3302	CG2	THR	690	18.808	43.736	75.355	1.00	24.38	6
ATOM	3303	C	THR	690	19.337	46.821	75.661	1.00	27.33	6
ATOM	3304	O	THR	690	20.052	47.436	74.841	1.00	25.88	8
ATOM	3305	N	ARG	691	19.653	46.704	76.966	1.00	28.66	7
ATOM	3306	CA	ARG	691	20.920	47.275	77.514	1.00	27.60	6
ATOM	3307	CB	ARG	691	20.908	47.426	79.055	1.00	28.38	6
ATOM	3308	CG	ARG	691	21.668	46.303	79.860	1.00	30.17	6
ATOM	3309	CD	ARG	691	21.736	46.597	81.403	1.00	30.51	6
ATOM	3310	NE	ARG	691	22.360	45.549	82.240	1.00	29.33	7
ATOM	3311	CZ	ARG	691	21.681	44.632	82.957	1.00	31.23	6
ATOM	3312	NH1	ARG	691	20.331	44.612	82.931	1.00	32.13	7
ATOM	3313	NH2	ARG	691	22.337	43.775	83.768	1.00	28.34	7
ATOM	3314	C	ARG	691	22.024	46.269	77.114	1.00	27.87	6
ATOM	3315	O	ARG	691	21.863	45.028	77.231	1.00	28.65	8
ATOM	3316	N	TYR	692	23.157	46.781	76.682	1.00	27.18	7
ATOM	3317	CA	TYR	692	24.223	45.893	76.256	1.00	23.54	6
ATOM	3318	CB	TYR	692	24.237	45.885	74.744	1.00	24.61	6
ATOM	3319	CG	TYR	692	23.317	44.905	74.100	1.00	23.60	6
ATOM	3320	CD1	TYR	692	23.303	43.575	74.501	1.00	23.69	6
ATOM	3321	CE1	TYR	692	22.544	42.636	73.833	1.00	23.82	6
ATOM	3322	CD2	TYR	692	22.535	45.283	73.014	1.00	24.04	6
ATOM	3323	CE2	TYR	692	21.755	44.345	72.325	1.00	24.91	6
ATOM	3324	CZ	TYR	692	21.772	43.022	72.745	1.00	24.40	6
ATOM	3325	OH	TYR	692	21.021	42.086	72.059	1.00	27.00	8
ATOM	3326	C	TYR	692	25.534	46.436	76.739	1.00	22.44	6
ATOM	3327	O	TYR	692	25.776	47.643	76.606	1.00	21.10	8
ATOM	3328	N	THR	693	26.382	45.567	77.302	1.00	19.16	7
ATOM	3329	CA	THR	693	27.711	45.989	77.758	1.00	14.99	6
ATOM	3330	CB	THR	693	27.877	45.985	79.301	1.00	13.81	6
ATOM	3331	OG1	THR	693	26.746	46.642	79.909	1.00	14.05	8
ATOM	3332	CG2	THR	693	29.125	46.745	79.685	1.00	12.28	6
ATOM	3333	C	THR	693	28.733	45.070	77.062	1.00	14.45	6
ATOM	3334	O	THR	693	28.450	43.870	76.926	1.00	11.01	8
ATOM	3335	N	PHE	694	29.811	45.661	76.604	1.00	15.34	7
ATOM	3336	CA	PHE	694	30.841	44.969	75.845	1.00	15.68	6
ATOM	3337	CB	PHE	694	30.833	45.501	74.405	1.00	18.12	6
ATOM	3338	CG	PHE	694	29.457	45.682	73.816	1.00	19.49	6
ATOM	3339	CD1	PHE	694	28.740	46.860	74.043	1.00	18.66	6
ATOM	3340	CD2	PHE	694	28.882	44.679	73.015	1.00	18.42	6
ATOM	3341	CE1	PHE	694	27.480	47.035	73.481	1.00	19.71	6
ATOM	3342	CE2	PHE	694	27.617	44.854	72.450	1.00	16.44	6
ATOM	3343	CZ	PHE	694	26.919	46.024	72.679	1.00	16.79	6
ATOM	3344	C	PHE	694	32.237	45.210	76.374	1.00	14.83	6
ATOM	3345	O	PHE	694	32.533	46.304	76.835	1.00	14.75	8
ATOM	3346	N	ALA	695	33.112	44.227	76.155	1.00	14.22	7

bref21c.pdb Thu Apr 25 12:27:47 1996 44

ATOM	3347	CA	ALA	695	34.532	44.271	76.533	1.00	14.58	6
ATOM	3348	CB	ALA	695	34.704	43.821	77.959	1.00	15.52	6
ATOM	3349	C	ALA	695	35.331	43.352	75.579	1.00	16.59	6
ATOM	3350	O	ALA	695	34.739	42.503	74.883	1.00	16.77	8
ATOM	3351	N	VAL	696	36.663	43.475	75.554	1.00	18.89	7
ATOM	3352	CA	VAL	696	37.475	42.637	74.640	1.00	18.54	6
ATOM	3353	CB	VAL	696	37.455	43.242	73.198	1.00	19.19	6
ATOM	3354	CG1	VAL	696	37.867	44.705	73.223	1.00	17.15	6
ATOM	3355	CG2	VAL	696	38.335	42.446	72.255	1.00	20.60	6
ATOM	3356	C	VAL	696	38.923	42.284	75.047	1.00	18.64	6
ATOM	3357	O	VAL	696	39.654	43.093	75.637	1.00	18.43	8
ATOM	3358	N	ARG	697	39.321	41.055	74.738	1.00	18.97	7
ATOM	3359	CA	ARG	697	40.675	40.563	75.050	1.00	18.67	6
ATOM	3360	CB	ARG	697	40.593	39.173	75.664	1.00	17.03	6
ATOM	3361	CG	ARG	697	39.772	39.078	76.889	1.00	15.40	6
ATOM	3362	CD	ARG	697	39.842	37.650	77.417	1.00	18.07	6
ATOM	3363	NE	ARG	697	39.077	36.676	76.632	1.00	17.47	7
ATOM	3364	CZ	ARG	697	38.722	35.467	77.081	1.00	19.24	6
ATOM	3365	NH1	ARG	697	39.061	35.078	78.309	1.00	20.70	7
ATOM	3366	NH2	ARG	697	38.014	34.643	76.318	1.00	18.93	7
ATOM	3367	C	ARG	697	41.625	40.494	73.818	1.00	18.98	6
ATOM	3368	O	ARG	697	41.180	40.255	72.677	1.00	19.20	8
ATOM	3369	N	ALA	698	42.926	40.660	74.077	1.00	17.10	7
ATOM	3370	CA	ALA	698	43.973	40.609	73.057	1.00	14.99	6
ATOM	3371	CB	ALA	698	44.816	41.858	73.146	1.00	15.98	6
ATOM	3372	C	ALA	698	44.838	39.366	73.296	1.00	14.49	6
ATOM	3373	O	ALA	698	45.073	38.999	74.432	1.00	16.90	8
ATOM	3374	N	ARG	699	45.349	38.753	72.234	1.00	13.57	7
ATOM	3375	CA	ARG	699	46.174	37.540	72.325	1.00	10.72	6
ATOM	3376	CB	ARG	699	45.229	36.331	72.392	1.00	12.04	6
ATOM	3377	CG	ARG	699	45.692	35.014	71.794	1.00	12.63	6
ATOM	3378	CD	ARG	699	46.738	34.349	72.665	1.00	20.39	6
ATOM	3379	NE	ARG	699	46.913	32.810	72.399	1.00	21.37	7
ATOM	3380	CZ	ARG	699	46.119	31.955	72.895	1.00	21.92	6
ATOM	3381	NH1	ARG	699	45.069	32.257	73.672	1.00	21.47	7
ATOM	3382	NH2	ARG	699	46.442	30.682	72.710	1.00	22.33	7
ATOM	3383	C	ARG	699	47.090	37.470	71.094	1.00	9.38	6
ATOM	3384	O	ARG	699	46.680	37.820	69.991	1.00	10.86	8
ATOM	3385	N	MET	700	48.355	37.109	71.282	1.00	8.21	7
ATOM	3386	CA	MET	700	49.263	37.029	70.140	1.00	7.21	6
ATOM	3387	CB	MET	700	50.724	36.955	70.551	1.00	6.01	6
ATOM	3388	CG	MET	700	51.322	38.292	70.963	1.00	5.33	6
ATOM	3389	SD	MET	700	52.092	39.250	69.678	1.00	9.84	16
ATOM	3390	CE	MET	700	51.368	40.792	69.955	1.00	8.49	6
ATOM	3391	C	MET	700	48.875	35.808	69.375	1.00	6.64	6
ATOM	3392	O	MET	700	48.609	34.755	69.939	1.00	6.32	8
ATOM	3393	N	ALA	701	48.849	35.943	68.069	1.00	7.50	7
ATOM	3394	CA	ALA	701	48.425	34.837	67.250	1.00	8.94	6
ATOM	3395	CB	ALA	701	47.605	35.361	66.065	1.00	7.41	6
ATOM	3396	C	ALA	701	49.483	33.855	66.779	1.00	9.12	6
ATOM	3397	O	ALA	701	50.679	34.165	66.639	1.00	9.86	8
ATOM	3398	N	GLU	702	48.980	32.669	66.491	1.00	10.01	7
ATOM	3399	CA	GLU	702	49.763	31.574	65.987	1.00	13.16	6
ATOM	3400	CB	GLU	702	48.971	30.275	66.108	1.00	15.92	6
ATOM	3401	CG	GLU	702	48.724	29.784	67.501	1.00	18.17	6
ATOM	3402	CD	GLU	702	48.597	28.284	67.507	1.00	21.01	6
ATOM	3403	OE1	GLU	702	47.904	27.731	66.611	1.00	22.10	8
ATOM	3404	OE2	GLU	702	49.233	27.652	68.377	1.00	24.81	8
ATOM	3405	C	GLU	702	50.126	31.770	64.510	1.00	13.07	6
ATOM	3406	O	GLU	702	49.560	32.617	63.802	1.00	12.10	8
ATOM	3407	N	PRO	703	51.106	30.986	64.037	1.00	14.95	7
ATOM	3408	CD	PRO	703	51.501	30.820	62.625	1.00	17.31	6
ATOM	3409	CA	PRO	703	51.782	30.007	64.899	1.00	14.84	6
ATOM	3410	CB	PRO	703	51.896	28.794	63.999	1.00	14.77	6
ATOM	3411	CG	PRO	703	52.252	29.467	62.635	1.00	19.35	6
ATOM	3412	C	PRO	703	53.150	30.488	65.409	1.00	13.50	6
ATOM	3413	O	PRO	703	53.801	29.774	66.157	1.00	15.09	8
ATOM	3414	N	SER	704	53.587	31.681	65.002	1.00	11.82	7
ATOM	3415	CA	SER	704	54.873	32.218	65.461	1.00	9.78	6
ATOM	3416	CB	SER	704	55.156	33.574	64.798	1.00	9.23	6
ATOM	3417	OG	SER	704	55.301	33.474	63.394	1.00	8.65	8
ATOM	3418	C	SER	704	54.860	32.386	67.003	1.00	11.09	6
ATOM	3419	O	SER	704	55.621	31.729	67.736	1.00	12.01	8
ATOM	3420	N	PHE	705	53.937	33.229	67.468	1.00	8.75	7
ATOM	3421	CA	PHE	705	53.767	33.532	68.857	1.00	3.52	6
ATOM	3422	CB	PHE	705	53.223	34.973	68.988	1.00	5.09	6
ATOM	3423	CG	PHE	705	54.159	35.924	68.184	1.00	7.49	6
ATOM	3424	CD1	PHE	705	53.696	36.417	66.957	1.00	8.92	6

bref21c.pdb Thu Apr 25 12:27:47 1996 45

ATOM	3425	CD2	PHE	705	55.446	36.284	68.611	1.00	8.54	
ATOM	3426	CE1	PHE	705	54.512	37.252	66.163	1.00	7.44	
ATOM	3427	CE2	PHE	705	56.270	37.115	67.833	1.00	4.91	
ATOM	3428	CZ	PHE	705	55.804	37.598	66.606	1.00	5.19	
ATOM	3429	C	PHE	705	52.783	32.591	69.505	1.00	5.11	
ATOM	3430	O	PHE	705	52.257	31.697	68.878	1.00	4.57	
ATOM	3431	N	GLY	706	52.634	32.751	70.809	1.00	8.69	
ATOM	3432	CA	GLY	706	51.728	31.956	71.622	1.00	7.99	
ATOM	3433	C	GLY	706	51.661	32.726	72.932	1.00	9.39	
ATOM	3434	O	GLY	706	52.345	33.739	73.069	1.00	9.05	
ATOM	3435	N	GLY	707	50.829	32.295	73.878	1.00	10.91	
ATOM	3436	CA	GLY	707	50.738	32.990	75.162	1.00	9.87	
ATOM	3437	C	GLY	707	49.465	32.823	75.977	1.00	7.80	
ATOM	3438	O	GLY	707	48.894	31.731	76.063	1.00	7.37	
ATOM	3439	N	PHE	708	48.993	33.927	76.540	1.00	7.59	
ATOM	3440	CA	PHE	708	47.801	33.911	77.372	1.00	8.42	
ATOM	3441	CB	PHE	708	48.171	33.981	78.874	1.00	9.14	
ATOM	3442	CG	PHE	708	49.358	33.126	79.277	1.00	8.19	
ATOM	3443	CD1	PHE	708	49.196	31.787	79.592	1.00	5.98	
ATOM	3444	CD2	PHE	708	50.638	33.679	79.352	1.00	6.32	
ATOM	3445	CE1	PHE	708	50.296	31.016	79.974	1.00	8.74	
ATOM	3446	CE2	PHE	708	51.730	32.912	79.731	1.00	5.05	
ATOM	3447	CZ	PHE	708	51.570	31.587	80.040	1.00	4.00	
ATOM	3448	C	PHE	708	46.846	35.066	77.077	1.00	7.99	
ATOM	3449	O	PHE	708	47.260	36.187	76.721	1.00	6.94	
ATOM	3450	N	TRP	709	45.562	34.777	77.285	1.00	9.09	
ATOM	3451	CA	TRP	709	44.475	35.752	77.119	1.00	12.14	
ATOM	3452	CB	TRP	709	43.114	35.083	77.396	1.00	11.59	
ATOM	3453	CG	TRP	709	42.417	34.592	76.165	1.00	12.07	
ATOM	3454	CD2	TRP	709	42.098	35.354	74.999	1.00	9.80	
ATOM	3455	CE2	TRP	709	41.465	34.481	74.092	1.00	9.82	
ATOM	3456	CE3	TRP	709	42.283	36.687	74.634	1.00	9.79	
ATOM	3457	CD1	TRP	709	41.971	33.326	75.929	1.00	11.53	
ATOM	3458	NE1	TRP	709	41.398	33.250	74.688	1.00	12.13	
ATOM	3459	CZ2	TRP	709	41.018	34.897	72.841	1.00	9.03	
ATOM	3460	CZ3	TRP	709	41.838	37.103	73.399	1.00	11.59	
ATOM	3461	CH2	TRP	709	41.214	36.209	72.513	1.00	10.54	
ATOM	3462	C	TRP	709	44.635	36.973	78.056	1.00	10.56	
ATOM	3463	O	TRP	709	44.770	36.823	79.268	1.00	12.13	
ATOM	3464	N	SER	710	44.620	38.177	77.508	1.00	11.52	
ATOM	3465	CA	SER	710	44.765	39.350	78.351	1.00	12.14	
ATOM	3466	CB	SER	710	45.040	40.594	77.501	1.00	9.78	
ATOM	3467	OG	SER	710	43.847	41.258	77.157	1.00	10.05	
ATOM	3468	C	SER	710	43.522	39.567	79.216	1.00	12.22	
ATOM	3469	O	SER	710	42.531	38.832	79.139	1.00	17.16	
ATOM	3470	N	ALA	711	43.580	40.563	80.076	1.00	12.01	
ATOM	3471	CA	ALA	711	42.435	40.867	80.894	1.00	12.49	
ATOM	3472	CB	ALA	711	42.855	41.817	81.993	1.00	12.98	
ATOM	3473	C	ALA	711	41.432	41.560	79.965	1.00	13.22	
ATOM	3474	O	ALA	711	41.810	42.073	78.915	1.00	14.99	
ATOM	3475	N	TRP	712	40.155	41.558	80.326	1.00	13.85	
ATOM	3476	CA	TRP	712	39.159	42.251	79.527	1.00	12.59	
ATOM	3477	CB	TRP	712	37.751	42.031	80.092	1.00	8.73	
ATOM	3478	CG	TRP	712	37.202	40.647	79.845	1.00	8.57	
ATOM	3479	CD2	TRP	712	36.796	40.091	78.576	1.00	8.04	
ATOM	3480	CE2	TRP	712	36.416	38.745	78.809	1.00	8.30	
ATOM	3481	CE3	TRP	712	36.718	40.600	77.270	1.00	4.78	
ATOM	3482	CD1	TRP	712	37.037	39.647	80.769	1.00	8.29	
ATOM	3483	NE1	TRP	712	36.574	38.499	80.150	1.00	8.70	
ATOM	3484	CZ2	TRP	712	35.969	37.906	77.783	1.00	8.46	
ATOM	3485	CZ3	TRP	712	36.279	39.776	76.262	1.00	7.52	
ATOM	3486	CH2	TRP	712	35.908	38.434	76.520	1.00	9.00	
ATOM	3487	C	TRP	712	39.498	43.747	79.520	1.00	12.59	
ATOM	3488	O	TRP	712	40.124	44.269	80.460	1.00	12.30	
ATOM	3489	N	SER	713	39.174	44.385	78.395	1.00	15.22	
ATOM	3490	CA	SER	713	39.366	45.819	78.166	1.00	15.45	
ATOM	3491	CB	SER	713	39.294	46.108	76.659	1.00	14.50	
ATOM	3492	OG	SER	713	37.973	45.899	76.149	1.00	21.86	
ATOM	3493	C	SER	713	38.167	46.480	78.799	1.00	15.66	
ATOM	3494	O	SER	713	37.081	45.908	78.764	1.00	18.64	
ATOM	3495	N	GLU	714	38.309	47.705	79.279	1.00	17.04	
ATOM	3496	CA	GLU	714	37.163	48.391	79.888	1.00	20.29	
ATOM	3497	CB	GLU	714	37.524	49.809	80.276	1.00	22.84	
ATOM	3498	CG	GLU	714	38.470	49.836	81.447	1.00	24.61	
ATOM	3499	CD	GLU	714	38.699	51.236	81.978	1.00	26.47	
ATOM	3500	OE1	GLU	714	39.860	51.479	82.420	1.00	27.51	
ATOM	3501	OE2	GLU	714	37.735	52.074	81.957	1.00	25.69	
ATOM	3502	C	GLU	714	35.885	48.366	79.027	1.00	21.46	

bref21c.pdb Thu Apr 25 12:27:47 1996 46

ATOM	3503	O	GLU	714	35.867	48.844	77.886	1.00 21.24	8
ATOM	3504	N	PRO	715	34.787	47.852	79.611	1.00 20.46	7
ATOM	3505	CD	PRO	715	34.703	47.767	81.090	1.00 21.13	6
ATOM	3506	CA	PRO	715	33.460	47.694	79.015	1.00 19.23	6
ATOM	3507	CB	PRO	715	32.627	47.183	80.182	1.00 21.32	6
ATOM	3508	CG	PRO	715	33.226	47.974	81.352	1.00 19.98	6
ATOM	3509	C	PRO	715	32.874	48.959	78.473	1.00 20.02	6
ATOM	3510	O	PRO	715	33.194	50.060	78.922	1.00 20.10	8
ATOM	3511	N	VAL	716	31.934	48.769	77.562	1.00 20.51	7
ATOM	3512	CA	VAL	716	31.229	49.858	76.910	1.00 19.78	6
ATOM	3513	CB	VAL	716	31.769	50.100	75.440	1.00 18.56	6
ATOM	3514	CG1	VAL	716	30.988	49.293	74.396	1.00 18.80	6
ATOM	3515	CG2	VAL	716	31.749	51.563	75.099	1.00 16.95	6
ATOM	3516	C	VAL	716	29.778	49.366	76.908	1.00 21.79	6
ATOM	3517	O	VAL	716	29.515	48.182	76.624	1.00 20.72	8
ATOM	3518	N	SER	717	28.859	50.269	77.264	1.00 22.27	7
ATOM	3519	CA	SER	717	27.439	49.971	77.331	1.00 21.09	6
ATOM	3520	CB	SER	717	26.920	50.181	78.764	1.00 23.89	6
ATOM	3521	OG	SER	717	27.182	49.064	79.607	1.00 24.17	8
ATOM	3522	C	SER	717	26.552	50.748	76.375	1.00 20.65	6
ATOM	3523	O	SER	717	26.541	51.970	76.394	1.00 19.78	8
ATOM	3524	N	LEU	718	25.838	50.014	75.523	1.00 21.29	7
ATOM	3525	CA	LEU	718	24.866	50.583	74.585	1.00 21.71	6
ATOM	3526	CB	LEU	718	25.009	49.949	73.188	1.00 17.72	6
ATOM	3527	CG	LEU	718	24.502	50.860	72.057	1.00 15.29	6
ATOM	3528	CD1	LEU	718	25.271	52.197	72.069	1.00 11.08	6
ATOM	3529	CD2	LEU	718	24.631	50.165	70.733	1.00 11.73	6
ATOM	3530	C	LEU	718	23.477	50.236	75.183	1.00 22.58	6
ATOM	3531	O	LEU	718	23.399	49.506	76.191	1.00 24.55	8
ATOM	3532	N	LEU	719	22.392	50.723	74.564	1.00 23.55	7
ATOM	3533	CA	LEU	719	21.023	50.470	75.054	1.00 23.37	6
ATOM	3534	CB	LEU	719	20.632	51.586	76.069	1.00 23.00	6
ATOM	3535	CG	LEU	719	21.540	51.746	77.325	1.00 22.19	6
ATOM	3536	CD1	LEU	719	21.290	53.039	78.084	1.00 19.79	6
ATOM	3537	CD2	LEU	719	21.416	50.545	78.254	1.00 20.88	6
ATOM	3538	C	LEU	719	19.986	50.393	73.904	1.00 23.18	6
ATOM	3539	O	LEU	719	18.886	50.958	74.036	1.00 24.17	8
ATOM	3540	N	THR	720	20.325	49.657	72.828	1.00 22.42	7
ATOM	3541	CA	THR	720	19.498	49.515	71.597	1.00 21.89	6
ATOM	3542	CB	THR	720	19.038	48.042	71.295	1.00 22.47	6
ATOM	3543	OG1	THR	720	18.798	47.332	72.513	1.00 24.25	8
ATOM	3544	CG2	THR	720	20.042	47.288	70.444	1.00 20.74	6
ATOM	3545	C	THR	720	18.263	50.417	71.492	1.00 22.94	6
ATOM	3546	O	THR	720	17.140	49.947	71.240	1.00 22.69	8

Table 1

Data Set	Resolution (Å)	Reflections (#)	Completeness	R_{sym}*	Sites	R_{iso}†	R_{Cullis}‡	R_{Kraut}	Phasing Power§
Native	25.0-2.8	14158	0.93(0.91)[a]	0.05	-	-	-	-	-
$HgAc_2$	25.0-3.0	11496	0.93 (0.91)	0.10	2	0.102	0.56	0.114¶ 0.100#	Iso 1.87 (3.1Å) Ano 1.35 (4.0Å)
$UO_2(NO_3)_2$	25.0-3.0	11931	0.96 (0.94)	0.14	4	0.116	0.62	0.137¶ 0.114	Iso 1.95 (3.1Å) Ano 1.72 (3.9Å)

Refinement Statistics:

Resolution (Å)	Relflections F>1σ	Total Number of atoms	R-value	RMS from ideal values: Bond Length	RMS from ideal values: Bond Angle	Average B Value (Å²): EBP1	EBP2	Peptides
8.0-2.8	13894	3462	0.21	0.016(Å)	2.1°	10.5	12.3	10.7

*$R_{sym}=\Sigma|I-\langle I\rangle|/\Sigma I$.

†$R_{iso}=\Sigma|F_{PH}-F_P|/\Sigma F_P$.

‡$R_{Cullis}=\Sigma||F_{PH}\pm F_P|-F_{H(calc)}|/|F_{PH}-F_P|$ for all centric reflections.

¶$R_{Kraut}=\Sigma||F_{PH(obs)}-F_{PH(calc)}|+|F^{+}_{PH(obs)}-F^{+}_{PH(calc)}||/\Sigma(F^{+}_{PH(obs)}+F^{-}_{PH(obs)}$ for all acentric relfections (anamalous case).

§Phase Power=$\{\Sigma|F_{PH(calc)}|^2/\Sigma|F_{PH(obs)}-F_{p(calc)}|^2\}^{1/2}$; $|F_{PH(obs)}-F_{P(calc)}|$ is the lack of closure error to maximum resolution indicated.

Mean Figure of Merit=$\langle|\Sigma P(\alpha)e^{i\alpha}/\Sigma P(\alpha)|\rangle$ where $P(\alpha)$ is the phase probability.

[a]Completeness of data in the outer shell, (2.9-2.8Å) for the native and (3.1-3.0Å) for both derivatives.

Table 2

Peptide1-EBP1	Peptide1-EBP2	Peptide1-EBP2	Peptide2-EBP1	Peptide1-Peptide2
$Gly^{P9}O$-$Met^{150}N$	$Tyr^{P4}OH$-$Ser^{92}N$	Gly^{P9} O-$Met^{150}N$	$Tyr^{P4}OH$-$Ser^{92}N$	$Tyr^{P4}O$-$Cys^{P6}N$
$Pro^{P10}O$-$Thr^{151}N$		$Pro^{P10}O$-$Thr^{151}N$		$Tyr^{P4}N$-$Cys^{P6}O$
$Pro^{P10}O$-$Thr^{151}O\gamma$		$Pro^{P10}O$-$Thr^{151}O\gamma 1$		$Cys^{P6}O$-$Tyr^{P4}N$
$Leu^{P11}O$-$Ser^{152}N$		$Leu^{P11}O$-$Ser^{152}N$		$Cys^{P6}N$-$Tyr^{P4}O$
$Leu^{P11}O$-$Ser^{152}O\gamma$		$Leu^{P11}O$-$Ser^{152}O\gamma$		

CLAIMS

What is claimed is:

1. A computer-assisted method for identifying potential mimetics of erythropoietin, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:

(a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when said peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of said receptor, thereby generating a criteria data set;

(b) comparing, using said processor, said criteria data set to a computer database of chemical structures stored in said computer data storage system;

(c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said criteria data set;

(d) outputting to said output device the selected chemical structures having a portion similar to said criteria data set.

2. A computer-assisted method for identifying potential mimetics of erythropoietin, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:

(a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when said peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of said receptor, thereby generating a criteria data set;

(b) constructing, using computer methods, a model of a chemical structure having a portion that is structurally similar to said criteria data set;

(c) outputting to said output device the constructed model.

3. A compound having a chemical structure selected using the method of claim 1, said compound being an EPO mimetic.

4. The compound of claim 3 wherein said compound is not a peptide.

5. The compound of claim 3 wherein said compound is a peptide.

6. The compound of claims 5 wherein said peptide has 15 of fewer amino acids.

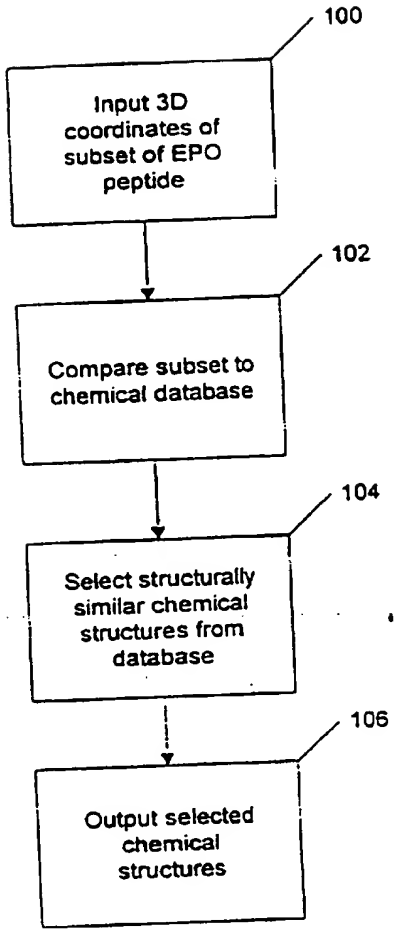

100
Input 3D coordinates of subset of EPO peptide
102
Compare subset to chemical database
104
Select structurally similar chemical structures from database
106
Output selected chemical structures

FIG. 1

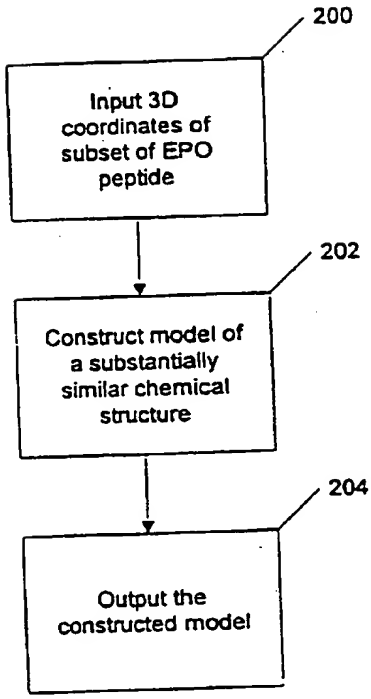

200
Input 3D coordinates of subset of EPO peptide
202
Construct model of a substantially similar chemical structure
204
Output the constructed model

FIG. 2

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US97/07218

A. CLASSIFICATION OF SUBJECT MATTER

IPC(6) :G06F 159:00
US CL :364/496

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 364/496, 497,498,578

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

aps, dialog
search terms: erythropoietin, receptor, 3d, pdb or database

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	US, 5,331,573 A (BALAJI et al.) 19 July 1994, (col. 7, lines 46-66, col. 13, lines 20-55, col. 14, lines 12-23	1-6
A,P	US 5,557,535 A (SRINIVASAN et al.) 17 September 1996, (abstract, fig. 1, col. 4, line 57 - col. 6,line 55)	1,2
A,P	US 5,555,366 A (TEIG et al.) 10 September 1996, (abstract, fig. 8, fig. 12)	1,2
A	US 5,265,030 A (SKOLNICK et al.) 23 November 1993, (col. 2, line 20 - col. 3, line 20)	1,2
A,P	MCCARTHY, "Small Peptide Designed that can Mimic Erythropoietin" Lancet, 8/96 vol. 348, no. 24, p.395	1-6

[X] Further documents are listed in the continuation of Box C. [ ] See patent family annex.

* Special categories of cited documents:

"A" document defining the general state of the art which is not considered to be part of particular relevance

"E" earlier document published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art

"&" document member of the same patent family

Date of the actual completion of the international search
05 JULY 1997

Date of mailing of the international search report
04 AUG 1997

Name and mailing address of the ISA/US
Commissioner of Patents and Trademarks
Box PCT
Washington, D.C. 20231
Facsimile No. (703) 305-3230

Authorized officer
MELANIE KEMPER

Telephone No. (703) 305-3900

Form PCT/ISA/210 (second sheet)(July 1992)*

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US97/07218

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X,P	LIVNAH ET AL., "Functional Mimicry of a Protein Hormone by a Peptide Agonist" Science 26 July 1996, vol. 273 no. 274, p. 464-471.	1-6